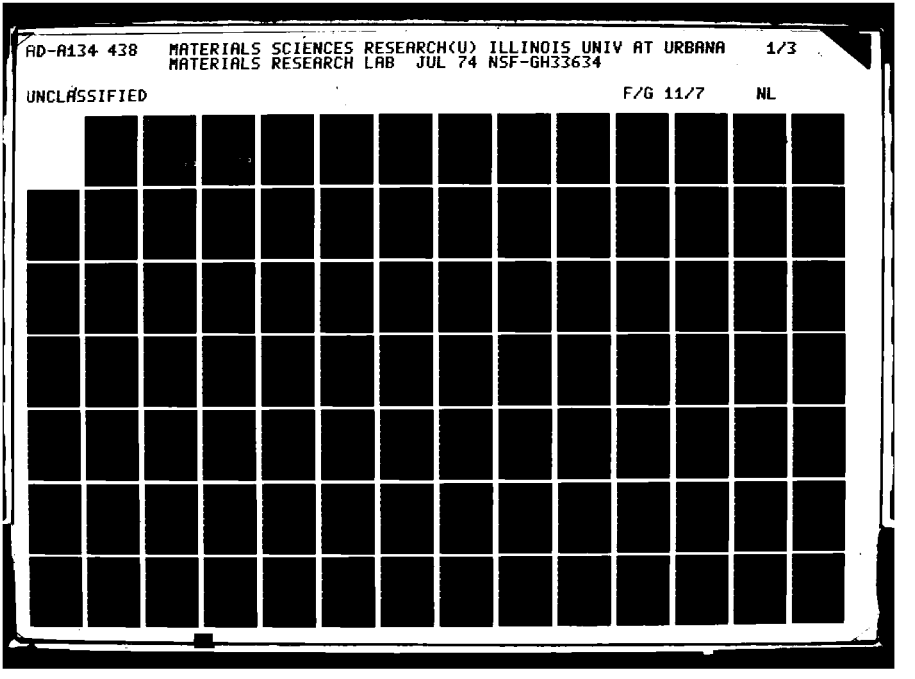
AD-A134 438 MATERIALS SCIENCES RESEARCH(U) ILLINOIS UNIV AT URBANA 1/3
MATERIALS RESEARCH LAB JUL 74 NSF-GH33634
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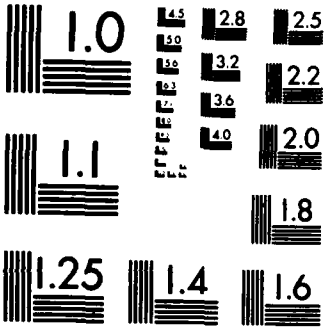

ANNUAL TECHNICAL REPORT

1973 - 1974

(July 1, 1973 thru June 30, 1974)

on

Materials Sciences Research

Submitted to the

NATIONAL SCIENCE FOUNDATION
(GH 33634)

by the

MATERIALS RESEARCH LABORATORY
UNIVERSITY OF ILLINOIS
URBANA, ILLINOIS

JULY 1974

This report lists the research output of all Materials Research Laboratory Project Principal Investigators. The research reported has been supported by the National Science Foundation, the Advanced Research Projects Agency, the U.S. Atomic Energy Commission, the U.S. Office of Naval Research, the U.S. Air Force Office of Scientific Research, and the U.S. Army Research Office.

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MATERIALS RESEARCH LABORATORY

ANNUAL TECHNICAL REPORT

1973-1974

TABLE OF CONTENTS

INTRODUCTION

The Materials Research Laboratory of the University of Illinois was established in June, 1962, as an interdepartmental and interdisciplinary laboratory of the College of Engineering. The following departments of the University participate in its operation:

Department of Ceramic Engineering
Department of Chemistry and Chemical Engineering
Department of Electrical Engineering
Department of Geology
Department of Metallurgy and Mining Engineering
Department of Physics

The administration of the Laboratory is the responsibility of an Administrative Staff and a Steering Committee. The Administrative Staff of the Laboratory is:

Robert J. Maurer, Professor of Physics, Director
John Stanley, Business Manager

The Steering Committee of the Laboratory is:

J. Bardeen, Professor of Electrical Engineering and of Physics
H. G. Drickamer, Professor of Chemical Engineering and of Physical Chemistry
A. L. Friedberg, Professor of Ceramic Engineering; Head, Department of Ceramic Engineering
R. O. Simmons, Professor of Physics; Head, Department of Physics
C. A. Wert, Professor of Metallurgical Engineering; Head, Department of Metallurgy and Mining Engineering
R. J. Maurer, Professor of Physics (ex-officio)

During the past year an External Advisory Committee was appointed to advise the Director and Steering Committee concerning the quality of the research program, the wisdom of the choice of research directions, the functioning of the Central Facilities, and the appropriateness of the organization and administration. The members of the External Advisory Committee are:

M. Nevitt, Argonne National Laboratory
A. Overhauser, Purdue University
R. Oriani, U. S. Steel Corporation, Chairman
C. A. Swenson, Iowa State University

The scientific staff of the Laboratory consists of selected members of the participating departments and their graduate students. Laboratory staff members and programs are selected annually by the Steering Committee after a review of proposals submitted to the Director by faculty members of the participating departments.

The primary support for the Laboratory is derived from contracts and grants of the National Science Foundation, the U. S. Atomic Energy Commission and the Advanced Research Projects Agency with the University of Illinois.

Since July 1, 1973, the scientific program of the Laboratory has consisted of 40 projects of which 18 were supported by NSF, 16 were supported by AEC funds, and 6 were supported by ARPA funds. The number of senior staff members, excluding postdoctoral members, was 50. The number of postdoctorals was 26; of these 11 were supported by NSF, 6 were supported by AEC, 4 were supported by ARPA, and 5 received other support. A total of 118 graduate students were supported by Research Assistantships; 37 by NSF, 56 by AEC, and 25 by ARPA. The number of graduate students supported by fellowships and associated with Laboratory projects was 16 and there were 5 teaching assistants who were directly associated with MRL projects.

There are 8 professional staff members whose appointments are in the Laboratory and who assist Laboratory projects and facilities with technical assistance. Mr. Ian Ward will join the professional staff in June 1974 to assist Mr. John Woodhouse with the operation of the Electron Microscope Facility.

Twenty-nine Ph.D. theses were completed and degrees granted with Laboratory support for the period July 1, 1973 - June 30, 1974; there were 5 Masters degree theses. The titles of these theses, the names of the students, and the dates of the award of the degrees are given on pages 189-192 and are included in the individual project technical reports.

For the period July 1, 1973 - June 30, 1974, the number of publications which received Laboratory support is 147. Of these publications, 64 received NSF support, 30 were NSF-ARPA supported, 2 were NSF-AEC supported, 16 were supported by ARPA, 34 were supported by AEC and 1 was AEC-NSF-ARPA supported. In addition, there are 104 papers in process of publication at this time.

New Projects

Hamish L. Fraser, Assistant Professor of Metallurgy
Deformation of Intermetallic Compounds at Elevated Temperatures
Supported by the U. S. Atomic Energy Commission

A. Barry Kunz, Professor of Physics
Electronic Structure of Solids
Supported by the National Science Foundation

William McMillan, Professor of Physics
Research on the Dynamic Structure of Liquids, Liquid Crystals, and Disordered Solids
Supported by the Advance Research Projects Agency

Terminated Projects

Frederick C. Brown, Professor of Physics
Ultraviolet Response of Solid Thin Films
Supported by the National Science Foundation

Paul Handler, Professor of Physics and Electrical Engineering
Optical Properties of Solids
Supported by the National Science Foundation

Dillon E. Mapother, Professor of Physics
Thermodynamic Properties of Materials
Supported by the National Science Foundation

Joint MRL-Department Seminars

Ceramics-MRL Seminar
May 17, 1973
Diffusion in Some Transition Metal Oxides
Dr. J. Bruce Wagner, Jr., Department of Materials Science and Materials Research Center, Northwestern University

Metallurgy-MRL Seminar
May 23, 1973
Magnetism Specific Heat and Resistivity of Ni^3Al and Ni^3Ga
Dr. P. DeSchatel, University of Amsterdam, Holland

Metallurgy-MRL Colloquium
August 23, 1973
"M" The Rate Theory of Point Defect Aggregation in Irradiated Material
Dr. R. Bullough, Atomic Energy Research Establishment, Harwell, England

Solid State Physics-Ceramic Engineering-MRL Seminar
October 5, 1973
Metal-Insulator Transitions in Transition-Metal Oxides
Professor J. Honig, Purdue University

MRL Seminar
February 4, 1974
Ion Microprobe Analysis of Materials
Dr. James G. Bradley, NASA-Johnson Space Center, Houston, Texas

Physical Chemistry-MRL Seminar
February 6, 1974
Theory of Chemisorption
Professor Robert J. Schreiffer, University of Pennsylvania

MRL Seminar
March 21, 1974
The Precipitation of Zirconium Hydride
Dr. Graham Carpenter, Chalk River Nuclear Laboratory, Chalk River, Canada

MRL Seminar
April 1, 1974
Surface and Thin Film Analysis by High Energy (2MeV) Ion Scattering Spectrometry
Dr. W. K. Chu, Department of Electrical Engineering, California Institute of Technology, Pasadena

Physics-MRL Seminar
March 29, 1974
The Structure of Jupiter (H_2 and He Under Extreme Pressure)
Dr. R. Smoluchowski, Princeton University

Physical Chemistry - MRL Seminar
April 17, 1974
NMR of Dilute Spins; Applications to Chemistry and Biochemistry
Professor John Waugh, Department of Chemistry, Cambridge, Mass. (MIT)

Visiting Staff Members

Dr. A. M. Stoneham, U.K. Atomic Energy Research Establishment, Harwell, England, visited the Laboratory and consulted with Professor C. P. Flynn, May through October of 1973.

Dr. V. Van Doren, on leave from the University of Antwerp, Belgium, was associated with Dr. A. B. Kunz of the Department of Physics from December 1, 1973 through February 14, 1974.

Dr. S. Radhakrishna of the Indian Institute of Technology, Madras, India, was associated with Professor M. V. Klein of the Department of Physics, November 4 through December 22, 1973.

Valters Ziraps, IREX Soviet Scholar, of Latvian SSR was associated with Professor M. V. Klein of the Department of Physics from September 15, 1973 to May 22, 1974.

Dr. Ian Philip Jones of Birmingham University, England, was a Visiting Research Assistant Professor from September 21 through November 20, 1973, working with Dr. H. Fraser of the Department of Metallurgy and Mining Engineering.

Professor Fred M. Erensberger (from PPG Labs) is a Visiting Professor in the Department of Ceramic Engineering, working with Professor C. Bergeron.

Dr. R. Schwarz of the University of Virginia is a Visiting Assistant Professor in the Department of Physics and associated with Professor A. V. Granato.

E. E. Pollock, IBM Postdoc Fellow, arrived at the Laboratory October 1973 and is working with Professor Flynn's group (Physics) and C. Wert (Metallurgy).

Other Vistors

Dr. Werner Schilling, Julich, Germany, was a visitor at the Materials Research Laboratory, April 30 and May 1, 1973.

Dr. P. Dedericks, Institut fur Festhorbergorchung, Julich, Germany, visited the Laboratory May 15-17, 1973.

Dr. Tetsuzuki, Yokohama University, Yokohama, Japan, visited the Laboratory and consulted with Professor A. V. Granato of the Physics Department, July, 1973.

Prof. Dr. E. V. Franck, Inst. fur physik & electro. Chemie, University of Karlsrueh, West Germany, consulted with Professor H. G. Drickamer, August 7-9, 1973.

Dr. M. H. Loretto, University of Birmingham, England, visited the Laboratory and consulted concerning activities in the field of electron microscopy technicians, November, 1973.

Professor S. Bhagavantam, Indian Institute of Technology, Bangare, visited the Laboratory and consulted with Professor R. J. Maurer, December 17, 1973.

Professor Erwin G. Herlitzius, Technische, Universitat Dresden, and Dr. Herbert Friedrich, Zentralinstitut fur Elektronenphysik, Akademie der Wissenschaften, Berlin, visited Professors R. O. Simmons, C. T. Sah, M. V. Klein, and J. Bardeen on February 25, 1974. Our East German colleagues' mission is to visit several major universities to ascertain their suitability as sites for visits of scientists and engineers under IREX auspices.

Professor P. Krishna, Banaras Hindu University, Varanasi, India, visited the Laboratory May 23, 1974, to discuss structure of SiC and mechanisms of transformations between polytypes.

Honors and Awards

Professor A. C. Anderson, Department of Physics, became a member, U. S. National Committee for International Institute of Refrigeration, and Vice President, Commission A1, International Institute of Refrigeration (1974).

Professor John Bardeen, Departments of Physics and Electrical Engineering, was named "Illinoisan of the Year" by the Illinois News Broadcasters Association. He received the James Madison Medal, Princeton University (1973); Doctor of Science, Harvard University (1973); Foreign Member, Royal Society of Great Britain (1973): and received an honorary degree from the University of Illinois (1974).

Professor Paul Beck, Department of Metallurgy and Mining Engineering, has been named first recipient of the new Hume-Rothery Award from the Metallurgical Society of the AIME. The award is to be given annually to the outstanding research in the area of magnetism and electrical properties of alloys. (May 1974).

Professor Beck will receive the 1976 Sauveur Achievement Award at the ASM Awards and Fellow Convocation in Cleveland on October 19, 1976, during the Materials Engineering Congress. This award recognizes pioneering metallurgical achievements.

Professor Harry G. Drickamer, Department of Chemical Engineering, won the 1974 Irving Langmuir Award in Chemical Physics for his research in the electronic behavior of solids. (April 1974).

Professor Willis H. Flygare, Department of Chemistry, was recipient of the Fifteenth Leo Hendrik Baekeland Award, presented by the North Jersey Section, American Chemical Society, in recognition of his original and distinguished contribution to high resolution microwave spectroscopy, the molecular Zeeman effect, radio-astronomy, and molecular electro-optics. (October 1973).

Professor Flygare was elected to membership in the National Academy of Science (April 1974) and was elected Fellow of the American Academy of Arts and Sciences (May 1974).

The 1973 Stanley H. Pierce Award, University of Illinois, for development of student-faculty empathy and cooperation went to Professor Arthur L. Friedberg, Head of the Department of Ceramic Engineering and a Member of the MRL Steering Committee.

Professor Jon Holder, Department of Geology, has been invited to participate as a Visiting Consultant to the APA Energy Study Planning Committee at Brookhaven National Laboratory, June 17-18, 1974.

Professor Robert Maurer, Director of the Laboratory, was appointed to the Solid State Sciences Committee, National Academy of Sciences, National Research Council (1974) and was also appointed a member of the Council for International Exchange of Scholars, National Research Council (1974).

Professor David Pines of the Department of Physics has been elected to the National Academy of Sciences (1973); was a Visiting Scientist, Academy of Sciences (Peoples Republic of China: Visits to Canton, Peking, Dalian, Shen Yang, Shanghai, Changsha, as invited guest of Chinese Academy of Sciences (July 1973)); Editor, Reviews of Modern Physics (1973).

Two professors from the Department of Physics have been elected to positions in the American Physical Society. R. O. Simmons became the vice-chairman-elect of the Division of Solid State Physics of the APS. The position leads to vice-chairman and chairman in succeeding years. David Lazarus will serve a four-year term on the APS governing council.

Professor Charles P. Slichter, Department of Physics, was Chairman, President's Committee on the National Medal of Science; became member of Corporation, Harvard University, and became member of Corporation and Trustee, Woods Hole Oceanographic Institution.

Professor C. A. Wert, Department of Metallurgy and Mining Engineering, received the Alumni Achievement Award from Morningside College, Iowa, May 1974.

Gerald P. Wirtz, Associate Professor of Ceramic Engineering, was named to the half-time revolving assistant deanship in the College of Engineering, University of Illinois, for 1973-74.

Mr. Daniel Petty, a graduate student of the Department of Ceramic Engineering and a research assistant of the Materials Research Laboratory, won the Ceramographic Exhibit Prize in the category of Scanning Electron Microscopy at the Annual Meeting of the American Ceramic Society, Chicago, April 28 - May 1, 1974, for his entry "Dental Enamel" which consisted of micrographs of etched human dental enamel showing the microstructure of enamel prisms. This research was supported by the U. S. Atomic Energy Commission. Mr. Petty's thesis advisor is Dr. Wendell Williams, Professor of Ceramic Engineering and Physics.

Leaves of Absence

Professor Donald M. Ginsberg, Department of Physics, is on sabbatical leave for II Semester 1973-74 at the Physics Department, University of California, LaJolla.

Special Events

October 10-11, 1973 - Annual Review of AEC Program

November 29-30, 1973 - Informal workshop on "Solid State Theory and Materials Science", organized by A. B. Kunz

March 14-15, 1974 - MRL Directors Meeting

LABORATORY FACILITIES

Central Facilities

General changes were made in the organization of the Laboratory Facilities during the past year in order to improve their effectiveness. These changes are noted in the description of individual facilities. Some noteworthy additions to the facilities and certain changes in personnel of the professional staff are also included in these descriptions.

1. Machine and Faculty-Student Shop

This well-equipped shop employs nine Instrument Makers and Laboratory Mechanics. An area equipped with lathes, drill presses, mills, hand tools, is reserved for use by faculty and students.

Committee: F. Wise, H. Stapleton

2. Computer System

A Sigma 5 Computer with 12 time sharing terminals is equipped with a card reader, magnetic tape drive, a paper tape reader, and punch, a medium speed printer and a graphical Calcomp plotter. An addition of 32,000 words was made to the memory during the past year; the memory capacity is 96,000 words. There is 100 megabytes of magnetic disc storage. Also, a Texas Instruments, Inc., graphical time sharing terminal was added to the system during the past year. Dr. Russell Marshall is responsible for operations and is assisted by Mrs. V. Metze, Research Programmer, and four part time student operators.

Committee: A. B. Kunz, R. Marshall, M. Salamon, G. Stucky

3. Chemical Analytical Laboratory

This laboratory is concerned, primarily, with trace analysis for characterization of materials. The instrumentation includes an AEI MS7 mass spectrograph, an AEI ion microprobe, a Baird 3 meter optical spectrograph, a Jarrell-Ash atomic absorption apparatus, a flame photometer, a polarograph, and accessories. There is a laboratory for handling radioactive samples which is connected by a pneumatic tube with the neighboring Triga reactor for fast transport of samples from the reactor to the laboratory.

Dr. C. A. Evans, Senior Research Chemist, is responsible for operation of the Laboratory. He is assisted by Mr. R. Blattner, M.S., Research Chemist, Mrs. J. Baker, B.A., Assistant Research Chemist, and Mrs. C. Silber, B.A., Assistant Research Chemist. Mr. Blattner has replaced Mr. James Wolcott who left during the past year for an industrial position as did Dr. Bruce Colby.

Committee: C. A. Evans, G. DePasquali

4. Microstructure Laboratory

The former Electron Microscope Laboratory, Microprobe Laboratory, X-Ray Laboratory, and Metallographic Laboratory have been consolidated into this unit.

A JEOL 200 kilovolt electron microscope was added to the instrumentation during the past year which also includes a Hitachi HU-11A 100 kilovolt electron microscope, an ARL EMX electron probe microanalyzer, a JSM-03 Scanning Electron Microscope, two x-ray stations with a Laue back reflection camera and x-ray diffractometer, and a Zeiss metallograph with grinding and polishing equipment.

Mr. J. Woodhouse, B.A., Research Microprobe Analyst, is responsible for operation of the Laboratory with part time student assistance.

Committee: C. Wert, H. Fraser, J. Woodhouse

5. Optical Laboratory

The former Spectrophotometric and Raman Laboratories have been combined into this unit. The instrumentation comprises Beckman IR-9 and IR-11 infrared spectrophotometers, Cary 14R and 15 ultraviolet spectrophotometers and a Spec 1401 double monochromator with lasers and electronics for Raman scattering research.

Committee: M. Klein

6. Mechanical Test Laboratory

This facility contains a Model 810 Materials Testing System for tensile tests.

Committee: C. Altstetter

7. High Temperature Laboratory

This facility provides a variety of furnaces and ovens for general use. There are two vacuum furnaces and dilatometer.

Committee: S. Brown

8. Toxic Materials Laboratory

A chemical hood, dry box, and sink constructed for use with toxic inorganic materials are contained in a room with provision for filtered air exchange.

Committee: S. Brown

9. Crystal Growth Laboratory

This is a specialized facility with two vacuum systems capable of 10^{-6} and 10^{-11}Torr for the purification, zone refining, and crystal growth of refactory metals at high temperatures.

Committee: H. Birnbaum

10. *Accelerator Laboratory*

A 3 MEV Van de Graaf accelerator is housed in a shielded area with provision for electron and proton irradiation of materials.

Committee: J. Koehler

11. Cryogenic Laboratory

Fifteen stations are provided for cryostats with vacuum lines and pumps. There is provision for recovering and purifying helium. Special rails and trenches facilitate the handling of large dewar vessels and electromagnets. Liquid helium is provided by an A.D. Little liquifier which is separately housed and operated by the Department of Physics.

Committee: D. Ginsberg

12. Magnet Facility

Two superconducting magnets are available. One has a capability of 125 kilogauss and the other provides 70 kilogauss with a homogeneity of better than 10 parts per million over a volume of 1 cubic centimeter.

Committee: F. Brown, C. P. Slichter

13. Reading Room

A small collection of reference works, including Chemical Abstracts, is provided for general use.

Committee: R. Maurer

MATERIALS RESEARCH LABORATORY PROJECTS

This listing is divided into projects supported by NSF funds, projects supported by AEC funds, and projects supported by ARPA funds. Projects are listed by the name of the principal investigator, his departmental title, and project title.

National Science Foundation

Anderson, Ansel C., Professor of Physics
Experimental Research on the Properties of Materials at Very Low Temperatures

Bardeen, John, Professor of Physics and of Electrical Engineering
Theory of the Condensed State of Matter

Bergeron, Clifton, G., Professor of Ceramic Engineering
Nucleation and Crystal Growth in Simple Glass Systems

Brown, Theodore L., Professor of Chemistry
Nuclear Quadrupole Resonance and Spectroscopic Studies

Curtin, David Y., Professor of Chemistry
Reactions of Crystalline Organic Compounds in the Solid State

Dow, John D., Associate Professor of Physics
Electron-Phonon Interactions in Simple Metals

Evans, Charles A., Jr., Senior Research Chemist, Materials Research Laboratory
Mass Spectroscopy, Spectrochemistry Research

Flynn, Colin P., Professor of Physics
Electronic Structure of Metallic Alloys

Ginsberg, Donald M., Professor of Physics
Experimental Studies of Superconductors

Handler, Paul, Professor of Physics and Electrical Engineering
Optical Properties of Solids

Holder, Jon T., Assistant Professor of Geology
Mechanical and Thermal Properties of Solids

Kunz, A. Barry, Associate Professor of Physics
Electronic Structure of Solids

Mapother, Dillon E., Professor of Physics
Thermodynamic Properties of Materials

Mochel, Jack M., Associate Professor of Physics
Investigations of Cooperative Phenomena at Low Temperatures

Salamon, Myron B., Associate Professor of Physics
Properties of Magnetic Materials

Stapleton, Harvey J., Professor of Physics
Spin-Lattice Relaxation and Dynamic Nuclear Orientation

Stucky, Galen D., Professor of Inorganic Chemistry
Diffraction Studies of Solids

Wirtz, Gerald P., Associate Professor of Ceramic Engineering
Physical and Catalytic Properties of Oxides

Advanced Research Projects Agency

Flygare, Willis H., Professor of Chemistry
Light Scattering in Solutions of Polymers, Macromolecules, Dense Gases, Liquids, and Liquid Crystals

Holonyak, Nick, Jr., Professor of Electrical Engineering
Luminescence, Lasers, Carrier and Impurity Effects in Compound Semiconductors

Jonas, Jiri, Professor of Chemistry
High-Pressure Nuclear Magnetic Resonance and Raman Study of the Dynamic Structure of Liquids, Disordered Solids and Polymers

Klein, Miles V., Professor of Physics
Light Scattering from Disordered Materials

McMillan, William, Professor of Physics
Liquid Crystals and Phase Transitions

Sah, Chih-Tang, Professor of Electrical Engineering and of Physics
Properties of Recombination Centers in Semiconductors

Atomic Energy Commission

Altstetter, Carl J., Professor of Physical Metallurgy
Interstitial Solid Solutions

Beck, Paul A., Professor of Physical Metallurgy
Electronic Structure and Magnetism of Transition Metal Alloys

Birnbaum, Howard K., Professor of Physical Metallurgy
Point Defect - Dislocation Interactions

Drickamer, Harry G., Professor of Chemical Engineering and Physical Chemistry
Use of Very High Pressure to Investigate the Structure of Matter

Fraser, Hamish L., Assistant Professor of Metallurgy
Deformation of Intermetallic Compounds at Elevated Temperatures

Granato, Andrew V., Professor of Physics
Anharmonic Effect in Solids

Koehler, James S., Professor of Physics
Radiation Damage in Solids

Lazarus, David, Professor of Physics
Defect and Electronic Properties of Solids

Metzger, Marvin, Professor of Physical Metallurgy
Deformation of Reinforced Metals

Pugh, E. Neville, Professor of Metallurgical Engineering
The Mechanism of Stress-Corrosion Cracking: Propagation Studies

Rowland, Theodore J., Professor of Physical Metallurgy
Nuclear Magnetic Resonance Studies

Simmons, Ralph O., Professor of Physics; Head, Department of Physics
Properties of Noble Gas Crystals

Slichter, Charles P., Professor of Physics
Nuclear Magnetic Resonance in Solids

Wayman, C. Marvin, Professor of Metallurgical Engineering
Solid State Phase Transformations and Thin Films

Wert, Charles A., Professor of Physical Metallurgy; Head, Department of Metallurgy and Mining Engineering
Precipitation in Refractory Metal Alloys

Williams, Wendell S., Professor of Physics, of Ceramic Engineering, and of Bioengineering
Physics of Refractory Materials

PROJECT TECHNICAL REPORTS
NATIONAL SCIENCE FOUNDATION

Experimental Research on the Properties of Materials at Very Low Temperatures

Principal Investigator: Ansel C. Anderson, Ph.D.
Professor of Physics

Supporting Agency: National Science Foundation

Senior Staff: Ansel C. Anderson, Professor
Stephen G. O'Hara, Research Associate

Junior Staff: Duane Jay Christy, Research Assistant
James T. Folinsbee, Research Assistant
Mikko Paalanen, Fellow
Gregory J. Sellers, Research Assistant

Objectives: (1) Experimental research on the properties of pure materials and those containing impurities and lattice defects (helium, normal and superconducting metals, amorphous and crystalline dielectrics); (2) A basic understanding of materials and phenomena important to low temperature technology.

Approach: Low temperatures are used to take advantage of the simplifications that occur in the physics of transport processes and other phenomena at such temperatures, and to provide as an experimental tool a source of very high frequency phonons.

Progress: (01 07 73 - 30 06 74) Transition Metal Superconductors. Most data related to the superconducting states of V, Nb, and Ta have been interpreted in terms of two superconducting energy gaps, a dominate gap associated with the electronic d-band and a second much smaller gap associated with the s-band. We have shown, however, that there is no

evidence for the smaller gap in thermal transport or the specific heat, that indeed there is no definitive evidence for a second gap in these transition metals. The two-gap model has also been extended to high field superconducting alloys, mainly because it was assumed to be an established fact that two gaps existed in Nb. This extrapolation is no longer possible, the existence of a second gap is unlikely and must be demonstrated in each individual superconductor.

Motion of Hydrogen in Niobium. Using phonon-scattering and specific heat measurements, we have discovered local modes or excitations associated with H or D solutes in V, Nb, and Ta. The large H-D isotope effect in Nb suggests that the excitation is mechanical rather than electronic in nature. The energies are 10^2-10^3 smaller than the smallest excitations thus far detected by neutron scattering in these hydride systems. An interpretation of these modes should lead to a better understanding of the important problem of H diffusion in bcc metals since the excitation is a probe of the local potential experienced by the solute.

Dislocation-Phonon Interaction. Using thermal transport measurements, we have shown in a variety of materials that localized modes or eigen states are associated with dislocations. The data generally are in good agreement with an elastic-string concept of a dislocation. In particular in Pb, the data and theory agree without utilizing any adjustable or undetermined parameter. These results support the use of the string model in interpreting the elastic and inelastic behavior of many materials.

Publications: (01 07 73 - 30 06 74)

A. C. Anderson
Low-Noise ac Bridge for Resistance Thermometry at Low Temperatures
Review of Scientific Instruments 44, 1475-1477 (1973)
Supported by the National Science Foundation under Grant GH-33634

J. T. Folinsbee and A. C. Anderson
Anomalous Kapitza Resistance to Solid Helium
Physical Review Letters 31, 1580-1581 (1973)
Supported by the National Science Foundation under Grant GH-33634

A. C. Anderson
Refrigeration and Thermometry Below 1 K
Applications of Cryogenic Technology (Scholium, New York, 1973) Vol. 5, p. 144
Supported by the National Science Foundation under Grant GH-33634

R. E. Peterson and A. C. Anderson
The Kapitza Thermal Boundary Resistance
Journal of Low Temperature Physics 11, 639-665 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

G. J. Sellers, A. C. Anderson, and H. K. Birnbaum
The Anomalous Heat Capacity of Superconducting Niobium
Physics Letters 44A, 173-174 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

A. C. Anderson and R. E. Peterson
Transport of Heat Between Electrons and Phonons in Copper Below 0.2 K
physics status solidi b, 56, 243 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

A. C. Anderson and S. G. O'Hara
The Lattice Conductivity of Niobium
Journal of Low Temperature Physics (submitted to)
Supported by the National Science Foundation under Grant GH-33634

S. G. O'Hara and A. C. Anderson
The Scattering of Thermal Phonons by Dislocations in Superconducting Aluminum
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

S. G. O'Hara and A. C. Anderson
Thermal Impedance Across Metallic and Superconducting Foils Below 1 K
Journal of Physics and Chemistry of Solids (submitted to)
Supported by the National Science Foundation under Grant GH-33634

G. J. Sellers, M. Paalanen, and A. C. Anderson
The Anomalous Heat Capacity of Superconducting Vanadium
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

S. G. O'Hara and A. C. Anderson
The Scattering of Thermal Phonons by Dislocations in Superconducting Lead and Tantalum
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

M. P. Zaitlin and A. C. Anderson
Thermal Conductivity of Deformed Germanium Below 1 K
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

G. J. Sellers and A. C. Anderson
Calorimetry Below 1 K: the Specific Heat of Copper
Review of Scientific Instruments (submitted to)
Supported by the National Science Foundation under Grant GH-33634

S. G. O'Hara, G. J. Sellers, and A. C. Anderson
The Influence of Hydrogen on the Thermal Conductivities of Superconducting Nb and Ta
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

G. J. Sellers, A. C. Anderson, and H. K. Birnbaum
The Anomalous Heat Capacities of Niobium and Tantalum below 1 K
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

A. C. Anderson
The Kapitza Resistance and Related Phenomena
Proceedings of European Physical Society Topical Conference on Liquid and Solid Helium (submitted to)
Supported by the National Science Foundation under Grant GH-33634

J. T. Folinsbee and A. C. Anderson
The Kapitza Resistance to a Variety of Metallic Surfaces below 0.2 K
Journal of Low Temperature Physics (submitted to)
Supported by the National Science Foundation under Grant GH-33634

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Theory of the Condensed State of Matter

Principal Investigator: John Bardeen, Ph.D.
Professor of Physics and of Electrical Engineering;
Member, Center for Advanced Study

Supporting Agency: National Science Foundation

Senior Staff: John Bardeen, Professor
Gordon Baym, Professor
David Pines, Professor
Partha Bhattacharyya, Research Associate
Roger A. Smith, Research Associate

Junior Staff: Charles Aldrich III, Research Assistant
James W. Bray, Research Assistant
Robert J. Meyer, Research Assistant

Objective: To investigate those aspects of theoretical solid state and low temperature physics which are concerned with surface physics, phase transitions, optical and photoconducting properties of insulators and semiconductors, magnetic alloys, superconductors, and liquid helium. Much of the theoretical research is parallel with and supports experimental investigations.

Approach: Many body theoretical concepts and techniques are used and computer calculations employed.

Progress: (01 07 73 - 30 06 74) Further theoretical work has been done to investigate the possibility of enhancing the superconducting transition temperature at the interface between a thin metallic film and an appropriate semiconductor. It is hoped to decrease the Coulomb repulsion of metallic electrons near the Fermi surface by virtual creation of electron-

hole pairs in the semiconductor. A deeper understanding is required of the dielectric response, $\varepsilon(q,\omega)$, of a semiconductor for general q and ω. Studies are underway in this direction.

A semi-phenomenological theory has been developed to estimate the excess conductivity from fluctuations in psuedo-one-dimensional systems just above the Peierls transition from a metallic to an insulating state. The estimated excess conductivity is not sufficient to account for the extraordinary conductivity peaks reported by Heeger et al. in some specimens of the organic salt TTF-TCNQ. Further work is in progress on the microscopic theory of conductivity associated with charge density waves in such systems.

The excitation spectrum of liquid helium (^{4}He) has been studied with use of the coherent potential method in order to better understand the dispersion at small wave vector. Another study involves the development of techniques for calculating thermodynamic properties of dense many-body systems from the fundamental interaction between the particles, with applications to liquid ^{3}He and ^{4}He. The calculations help to better understand the relative roles of mass and statistics in determining the properties of liquid helium. Initial work has been done on ways of defining and measuring appropriate parameters to describe the superfluid phases of ^{3}He.

In collaboration with Professor W. L. McMillan, work has been done on molecular theory of smectic C, B and H phases of liquid crystals.

In collaboration with Professor A. B. Kunz, some work has continued on the electronic structure of metals, ionic crystals and rare gas solids and on the interaction of hydrogen atom with a lithium metal surface.

Publications: (01 07 73 - 30 06 74)

David Allender, James Bray, and John Bardeen
A Reply on Comment of Inkson and Anderson on 'Model for an Exciton Mechanism of Superconductivity'
Physical Review B8, 4433 (1973)
Supported by the National Science Foundation under Grant GH-33634

R. J. Meyer and W. L. McMillan
A Simple Molecular Theory of the Smectic C, B and H Phases
Physical Review B9, 899-906 (1974)
Supported by the National Science Foundation under Grant GH-33634

John Bardeen
Electron-Phonon Interaction and Superconductivity
Cooperative Phenomena, edited by H. Haken and M. Wagner (Springer-Verlag, Berlin, 1973), pp. 63-78
Supported by the National Science Foundation under Grant GH-33634

John Bardeen
Superconducting Fluctuations in One-Dimensional Organic Solids
Solid State Communications 13, 357-359 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Army Research Office (Durham) under Contract DA-HC04-69-C-0007

David Allender, J. W. Bray, and John Bardeen
Theory of Fluctuation Superconductivity from Electron-Phonon Interactions in Psuedo-One-Dimensional Systems
Physical Review B9, 119-129 (1974)
Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Army Research Office (Durham) DA-HC04-69-C-0007

John Bardeen
Solid-State Physics: Accomplishments and Future Prospects
Physics 6, 165-190 (1973)
No Support Acknowledged

A. B. Kunz, D. J. Mickish, and P. W. Deutsch
On the Interaction of a Hydrogen Atom with a Lithium Metal Surface
Solid State Communications 13, 35-38 (1973)
Supported by the National Science Foundation under Grant GH-33634,
by the U. S. Army Research Office DA-HC04-68-C0007, and by the
Aerospace Research Lab. F33615-72-C-1506

Daniel J. Mickish and A. Barry Kunz
Energy Bands in LiF and Solid Ar
Journal of Physics C: Solid State 6, 1723-1733 (1973)
Supported by the National Science Foundation under Grant GH-33634,
by the U. S. Army Research Office DA-HC04-69-C0007, and by the
Aerospace Research Lab. F33615-72-C-1506

A. B. Kunz and D. J. Mickish
Energy Bands in LiH
Journal of Physics C: Solid State 6, 83-85 (1973)
Supported by the National Science Foundation under Grant GH-33634,
by the U. S. Army Research Office DA-HC04-69-C0007, and by the
Aerospace Research Lab. F33615-72-C-1506

A. Barry Kunz and Daniel J. Mickish
A Study of the Electronic Structure and the Optical Properties of the Solid
Rare Gases
Physical Review B8, 779-794 (1973)
Supported by the National Science Foundation under Grant GH-33634,
by the U. S. Army Research Office DA-HC04-69-C0007, and by the
Aerospace Research Lab. F33615-72-C-1506

F. K. Lamb, C. J. Pethick, and D. Pines
A Model for Compace X-ray Sources: Accretion by Rotating Magnetic Stars
The Astrophysical Journal 184, 271-289 (1973)
Supported by the National Science Foundation under Grant GP-25855

Y. Avini, J. N. Bahcall, P. C. Joss, N. A. Bahcall, F. K. Lamb,
C. J. Pethick, and D. Pines
Steady Energy Source in Her X-1?
Nature Physical Science 246, 36-37 (1973)
Supported by the National Science Foundation (Non-MRL)

David Pines, Christopher J. Pethick, and Fred K. Lamb
Models for Compact X-ray Sources
Annals of the New York Academy of Sciences 224, 237-260 (1973)
Supported by the National Science Foundation under Grants GP-25855
and GP-37485X

David Pines and Jacob Shaham
Quadrupolar Analysis of Storage and Release of Elastic Energy in the Earth
Nature Physical Science 243, 122-127 (1973)
Supported by the National Science Foundation and Aspen Center for Physics

David Pines and Jacob Shaham
Seismic Activity, Polar Tides and the Chandler Wobble
Nature 245, 77-81 (1973)
Supported by the National Science Foundation and Aspen Center for Physics

D. Q. Lamb, F. K. Lamb, and D. Pines
Soft Gamma-ray Bursts from Accreting Compact Objects
Nature Physical Science 246, 52-54 (1973)
Supported by the National Science Foundation (Non-MRL)

Jacob Shaham, David Pines, and Malvin A. Ruderman
Neutron Star Structure from Pulsar Observations
Annals of the New York Academy of Science 224, 190-205 (1973)
Supported by the Aspen Center for Physics

David Pines and Jacob Shaham
Free Precession of Neutron Stars
Nature 248, 483-486 (1974)
Supported by the National Science Foundation (Non-MRL)

Gordon Baym and Elliott Flowers
Pion Condensation in Neutron Star Matter: Equilibrium Conditions and Model Calculations
Nuclear Physics A222, 29-64 (1974)
Supported by the National Science Foundation under Grants GP-16886 and 40395

Gordon Baym
Pion Condensation in Nuclear Star Matter
Physical Review Letters 30, 1340-1342 (1973)
Supported by the National Science Foundation under Grant GP-16886

P. B. Visscher
Finite Temperature Properties of the Hubbard Model: Phase Separation
Proceedings of the Conference on Magnetism and Magnetic Materials, Boston 1973 (submitted to)
Supported by the National Science Foundation under Grant GH-33634

T. L. Gilbert, A. B. Kunz, and D. J. Mickish
Atomic vs Band Models for Interpreting the LiK Soft X-ray Absorption Peak in Lithium Halides
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634, by the U. S. Army Research Office, and by the Aerospace Research Lab.

Daniel J. Mickish, A. Barry Kunz, and Sokrates T. Pantelides
Electronic Structure and Optical Properties of Metallic Calcium
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634, by the U. S. Army Research Office DA-HC04-69-C0007, and by the Aerospace Research Lab. F33615-72-C-1506

T. C. Collins, D. Esterling, D. J. Mickish, and A. Barry Kunz
Comments on the Energy Band Structures of the Solid Rare Gas Mixtures
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Aerospace Research Lab. F33615-72-C-1506

Sokrates T. Pantelides, Daniel J. Mickish, and A. Barry Kunz
An AB Initio Study of the Electronic Properties of Magnesium Oxide
Solid State Communications (submitted to)
Supported by the National Science Foundation under Grant GH-33634, by the Aerospace Research Lab. F33615-72-C-1506, and by the U. S. Army Research Office DAHC04-69-C0007

Sokrates T. Pantelides, Daniel J. Mickish, and A. Barry Kunz
Correlation Effects in Energy-Band Theory
Physical Review (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-39811

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Elliott Galetin Flowers, Jr. (G. Baym, Adviser)
Neutrino Emission and Pion Condensation in Dense Matter. Part I. Neutrino Pair Emission in Dense Matter: A Many Body Approach. Part II. Pion Condensation in Nuclear and Neutron Star Matter
October 1973
Supported by the National Science Foundation and by the Advanced Research Projects Agency

Reginald Rutherford III (M. Wortis, Adviser)
Energy Density Correlation in the Three-Dimensional Ising Model
June 1973
Supported by the Advanced Research Projects Agency and by the National Science Foundation

Gilson Matheus Carniero (C. J. Pethick, Adviser)
Finite Temperature Contributions to the Thermodynamic Properties of a Normal Fermi Liquid
October 1973
Supported by the U. S. Army Research Office (Durham)

Nucleation and Crystal Growth in Simple Glass Systems

Principal Investigator: Clifton G. Bergeron, Ph.D.
Professor of Ceramic Engineering

Supporting Agency: National Science Foundation

Senior Staff: Clifton Bergeron, Professor
Fred M. Erensberger, Visiting Professor

Junior Staff: Wynn Herron, Research Assistant, Ingram-Richardson Corp.
Ananda H. Kumar, Research Assistant
Charles Leedecke, PPG Industries Fellow
Robert A. Rita, Research Assistant

Objectives: To further our understanding of the mechanism of nucleation and crystal growth in glass-forming systems. Recrystallized glasses, commonly termed "Glass-Ceramics", refer to that group of materials which are formed into shape in the vitreous state and are subsequently heat-treated to convert the glass to the crystalline or partially crystalline state. An enhancement of the physical, chemical, and electrical properties results. Glass-Ceramics are used as substrates and as insulation in hybrid electronic circuits, as catalyst supports for automotive exhaust systems, heat exchangers, as corrosion resistant materials for high temperature environments, and numerous other applications. An improved understanding of the crystallization process is important to this unique class of materials.

Approach: Hot stage cinemicrography techniques are being used to determine the growth rates of crystals from undercooled glass-forming melts. Measurements of the coefficient of viscosity of the melts and of their molar volumes are made at temperatures within and above the temperature range of crystal growth. These viscosity and density values reflect the

structural changes which occur in the melts. The effect of additions of small quantities of selected impurities on the growth rates and morphology of the growing crystals are also being studied. The electron microprobe is being used to determine the concentration gradients of impurities at the crystal-glass interface.

Progress: (01 07 73 - 30 06 74) The crystal growth rates of potassium octoborate grown from its melt have been determined over a 250 degree range of undercooling. Analysis of the kinetic data indicates that the growth occurs by a surface nucleation mechanism over the entire range of undercooling. A morphological change in the growing crystal occurs at about 70 degrees of undercooling and appears to be related to changes occurring in the melt structure and possible changes in the dimensions of the nucleus.

The free energy of activation for molecular transport at the interface during crystal growth of cesium hexaborate from its melt has been identified with the free energy barrier for viscous flow in the bulk melt calculated according to a modified form of the Eyring equation for viscosity. This has led to the identification of the crystal growth mechanism as that of a two-dimensional nucleation type up to undercoolings of about 130 degrees. The edge free energy of the crystals in contact with the melt, calculated from growth kinetic data, agreed closely with the value calculated using the Turnbull-Stavely relationship. The morphological features of the crystals grown at various undercoolings suggest that at large undercoolings the two-dimensional nucleation mechanism degenerates to a continuous growth mechanism.

Studies of the crystallization of fiberglass compositions have yielded information which is applicable to the solution of devitrification problems encountered in fiberglass manufacture. The rates of growth and of dissolution of anorthite, wollastonite, diopside, and tridymite were determined as a function of temperature and were related to selected changes in glass composition.

Publications: (01 07 73 - 30 06 74)

H. S. A. Kumar and C. G. Bergeron
Crystal Growth Mechanisms of $Na_2B_4O_7$ and PbB_4O_7 from Their Undercooled Melts
Journal of Crystal Growth 22, 58-60 (1974)
Supported by the National Science Foundation under Grant GH-33634

Suzanne R. Nagel and C. G. Bergeron
Crystallization of $Na_2B_4O_7$ from Its Melt
Journal of the American Ceramic Society 57, 129-132 (1974)
Supported by the National Science Foundation under Grant GH-33634, by the NDEA Title IV Fellowships, and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

H. S. A. Kumar and C. G. Bergeron
Viscosity-Volume Relationship in Liquids
Journal of Chemical Physics (submitted to)
Supported by the National Science Foundation under Grant GH-33634

A. J. Marlor, H. S. A. Kumar, and C. G. Bergeron
Crystallization of Cesium Hexaborate from Its Undercooled Melt
Physics and Chemistry of Glasses (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

A. J. Marlor, C. G. Bergeron, and H. S. A. Kumar
X-Ray Diffraction Data and Enthalpy of Fusion of $Cs_2B_6O_{10}$
Journal of the American Ceramic Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

R. A. Rita and C. G. Bergeron
Crystallization of Pb_2SiO_4
Journal of the American Ceramic Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

C. G. Bergeron and A. J. Marlor
Mechanism of Corrosion of Vitreous Coatings
Proceedings of PEI Technical Forum, April 1974 (to be published)
Supported by Ingram-Richardson, Inc.

M. S. Thesis: (01 07 73 - 30 06 74)

Roeland J. Ansems (C. G. Bergeron, Adviser)
Crystallization in Fiberglass Compositions
January 1974
Supported by the National Science Foundation under Grant GH-33634 and by Australian Consolidated Industries Fiberglass Ltd.

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Nuclear Quadrupole Resonance and Spectroscopic Studies

Principal Investigator: Theodore L. Brown, Ph.D.
Professor of Chemistry

Supporting Agency: National Science Foundation

Senior Staff: Theodore L. Brown, Professor
N. Y. Hsieh, Research Associate

Junior Staff: James Atwood, Research Assistant
Blaine Byers, Research Assistant
Patrick Ireland, U. of I. Fellow
Raymond Sweany, NSF Fellow

Objectives: (a) Determine transition element nuclear quadrupole resonance spectra. Correlate with other physical observables to clarify the nature of bonding in organometallic compounds and metal-containing compounds of biochemical interest. (b) Carry out detailed studies of the kinetics and stereochemistry of substitution and ^{13}CO exchange reactions in transition metal carbonyl compounds. (c) Develop matrix isolation techniques for observation of compounds of atomic metals and small metal atom clusters with small molecules, e.g., N_2, O_2, CO, or NO.

Approach: (a) Nuclear quadrupole double resonance spectrometers will be employed for detection of nqr spectra of elements of interest, with much higher sensitivity than heretofore. One of these employs adiabatic demagnetization in the lab frame, with cross relaxation, to detect a rare spin system using an abundant spin system. A second instrument under construction will employ pure quadrupole spin echo detection, of an abundant spin, double irradiation of the rare spin leads to loss of spin echo amplitude.

Further progress has been made in developing an apparatus for matrix isolation spectroscopy of metal atom-small molecule interactions, and matrix isolation studies of organometallic systems.

Progress: (01 07 73 - 30 06 74) (a) Substantial progress has been made in the construction of the two double resonance spectrometers. Final testing of the spin echo spectrometer is in progress, and it is anticipated that the instrument will be collecting new data within a short time. The adiabatic demagnetization experiment has required considerably more construction, but progress has been good; it is anticipated that the instrument will be operational about September 1974.

Nuclear quadrupole coupling constant data have been obtained for several compounds of the form $M(CO)_{5-x}L_x^n$, where M is Mn, Fe or Co, and n is -1, 0 or +1, respectively. The symbol L represents a phosphine or phosphite ligand, and x may vary from 0 to 5, although not all members of the series have been studied. These compounds have isoelectronic structures, and all involve the same type of five-coordinate geometry about the central metal. The nuclear quadrupole coupling constants have been determined by nqr (^{55}Mn, ^{59}Co) or Mössbauer (^{57}Fe) spectroscopies. The data permit estimations of the relative electric field gradients at the metal nuclei. These have been compared with values for field gradients calculated from Hartree-Fock SCF atomic functions for 3d and 4p electrons. The results suggest that changes in nuclear charge are responsible for the observed changes in field gradients, and that variations in configuration at the metal are of minor importance.

(b) We have made considerable progress on a careful study of the stereochemistry of ^{13}CO exchange in $Mn(CO)_5Br$ and $Re(CO)_5Br$. The exchange in these systems proceeds via a rate-determining dissociation of CO from the metal carbonyl. One of the most interesting and fundamentally important questions in reactions of this type, is the stereochemical behavior of the five-coordinate intermediate, and the nature of its electronic ground state. We have been able to show that the intermediate is partially fluxional, i.e., that it partially undergoes rearrangement in the short time interval before it reacts with the incoming CO. The fact that rearrangement is not complete indicates that the time required for the rearrangement is much longer than would have been predicted from the considerations previously applied to this problem. There is a possibility, as yet unsubstantiated, that the slowness of the rearrangement is associated with an electronic forbiddenness.

Progress has been made in the study of the substitution reactions of two metal hydride compounds, $HMn(CO)_5$ and $HRe(CO)_5$. These compounds, which serve as models for important catalytic systems, are very difficult to study, but initial results are encouraging. We have found that hydride migration, which is presumed to be the important rate-determining step in many reactions at metal-hydrogen centers, is much slower in $HRe(CO)_5$ than in $HMn(CO)_5$. The factors which influence the migratory aptitude of the hydrogen in this type of system are not known. In both systems, strong catalysis by trace impurities, as yet unidentified, has been seen.

Our results are surprising because it has been commonly asserted that the heavier metal hydride is the more reactive. We find that quite the opposite is the case.

Publications: (01 07 73 - 30 06 74)

Theodore L. Brown
The Chemistry of Metallic Elements in the Ionosphere and Mesosphere
Chemical Reviews 73, 645-667 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-30256X

William D. Covey and Theodore L. Brown
A Kinetic Study of Amine Substitution in $Mc(CO)_5$(Amine) Complexes
Inorganic Chemistry 12, 2820 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-30256X and by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

Randolph J. Guschl and Theodore L. Brown
Comparative Study of Base Interactions with Three Methylatocobalt (III) Chelate Complexes
Inorganic Chemistry 12, 2815 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-30256X and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

Randolph J. Guschl, Raymond S. Stewart, and Theodore L. Brown
Solvent and Alkyl Substituent Effects on the Kinetics of Base Exchange in Alkylbis (dimethylglyoximato) Cobalt (III)-Trimethylphosphite Complexes
Inorganic Chemistry 13, 417 (1974)
Supported by the National Science Foundation under Grants GH-33634 and GP-30256X

Thomas E. Boyd and Theodore L. Brown
Cobalt-59 Nuclear Quadrupole Resonance Spectra of Phosphine and Phosphite Substituted Cobalt Carbonyl Compounds
Inorganic Chemistry 13, 422 (1974)
Supported by the National Science Foundation under Grants GH-33634, GP-6396X, and GP-30256X

Robert A. LaRossa and Theodore L. Brown
Cobalt-59 Nuclear Quadrupole and Nuclear Magnetic Resonance Spectra of Cobaloximes
Journal of the American Chemical Society 96, 2072 (1974)
Supported by the National Science Foundation under Grants GH-33634 and GP-30256X

R. J. Guschl and Theodore L. Brown
Effects of Ligand Modifications on the Kinetics of Base Exchange in Methylatobis (diimine) Cobalt (III) Adducts
Inorganic Chemistry 13, 959 (1974)
Supported by the National Science Foundation under Grant GP-30256X

Cheryl D. Pribula, Theodore L. Brown, and Eckard Munck
Calculated and Observed Field Gradients in $[M(CO)_{5-x}P_x]^n$ Complexes
Journal of the American Chemical Society (submitted to)
Supported by the National Science Foundation under Grants GH-33634, GP-6396X, and GP-30256X

Theodore L. Brown
Cobalt-59 Nuclear Quadrupole Resonance Spectroscopy
Accounts of Chemical Research (submitted to)
Supported by the National Science Foundation under Grants GH-33634, GP-6396X, and GP-30256X

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Robert Anthony LaRossa (T. L. Brown, Adviser)
Nuclear Quadrupole Resonance Studies of Cobalt (III) Complexes
October 1973
Supported by the National Science foundation under Grant GH-33634

Cheryl Deckert Pribula (T. L. Brown, Adviser)
Spectroscopic Studies of Penta-Coordinate Organometallic Complexes
October 1973
Supported by the National Science Foundation under Grant GH-33634

James Edmonds Eaton (T. L. Brown, Adviser)
Kinetics and Mechanisms of Substitution Reactions of Alkyl-Group IV Metal Cobalt-Tetracarbonyls
October 1973
Supported by the National Science Foundation

Mary Ellen Phelen Switzer (T. L. Brown, Adviser)
The Reactivity and Magnetochemistry of Selected Metallocenes
October 1973
Supported by the National Science Foundation

Thomas Edgar Boyd (T. L. Brown, Adviser)
Chemistry and Bonding in Substituted Cobalt Carbonyl Complexes
October 1973
Supported by the National Science Foundation (Non-MRL)

Randolph J. Guschl (T. L. Brown, Adviser)
Ligand Exchange Studies of Methylatocobalt (III) Complexes
October 1973
Supported by the National Science Foundation (Non-MRL)

Richard Leonard Kieft (T. L. Brown, Adviser)
Nuclear Magnetic Resonance Studies of Organometallic Exchange Reactions
October 1973
Supported by the National Science Foundation (Non-MRL)

Reactions of Crystalline Organic Compounds in the Solid State

Principal Investigator: David Y. Curtin, Ph.D.
Professor of Chemistry

Supporting Agency: National Science Foundation

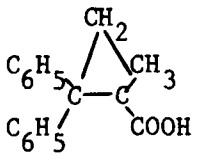
Senior Staff: David Y. Curtin, Professor
Chung-Tang Lin, Research Associate

Junior Staff: Gautam Desiraju, Teaching Assistant
Sherrill A. Puckett, Research Assistant

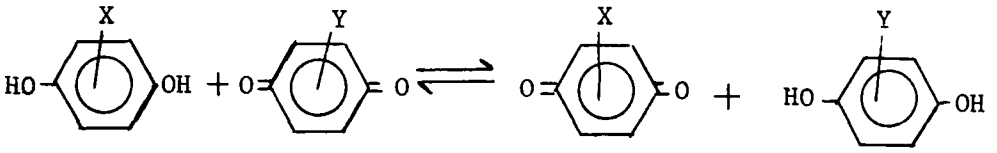
Objectives: To study chemical reactions of organic compounds in the solid state and of organic crystals with gases with the aim of determining the relationship between crystal structure and reactivity and particularly to use crystal forces to control chemical reactivity and chemical equilibria. This work is relevant to the technical utilization of organic compounds in industry.

Approach: Single crystals are studied using microscopic techniques and chemical analytical methods to study rates and products of thermally-induced reactions of single crystals and of reactions of crystals with gases.

Progress: (01 07 73 - 30 06 74) We have prepared in optically active form, determined the X-ray crystal structure [in collaboration with Dr. Iain C. Paul] and studied the reaction with ammonia gas of single crystals of the cyclopropanecarboxylic and acid below.



Preliminary solution studies of the oxidation-reduction equilibrium of appropriately substituted quinones and hydroquinones have shown that the exchange below can be studied by nmr techniques and is sufficiently slow to permit the isolation of isomeric complexes whose oxidation-reduction equilibria and other chemistry can be studied in the solid state.



Publications: (01 07 73 - 30 06 74)

Iain C. Paul and David Y. Curtin
Thermally Induced Organic Reactions in the Solid State
Accounts of Chemical Research 6, 217-225 (1973)
Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract HC-15-73-G10 by the Hoffman LaRoche Foundation, and by the National Institute of Health

David Y. Curtin
Stereo Pair Drawings of Crystal Structures Prepared by a Desk Calculator-Computer
Journal of Chemical Education 50, 775-778 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-34545X, and by the Advanced Research Projects Agency under Contract HC-15-73-G10

Chung-Tang Lin, Iain C. Paul, and David Y. Curtin
Anisotropic Reaction with Ammonia Gas of a Crystal of a Carboxylic Acid with Linear Hydrogen-Bonded Chains. An Example of Unitropic Attack
Journal of the American Chemical Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Rodger S. Miller, David Y. Curtin, and Iain C. Paul
Reactions of Molecular Crystals with Gases I. Reaction of Solid Aromatic Carboxylic Acids and Related Compounds with Ammonia and Amines
Journal of American Chemical Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Rodger S. Miller, Iain C. Paul, and David Y. Curtin
Reactions of Molecular Crystals with Gases II. The X-Ray Structure of Crystalline 4-Chlorobenzoic Acid and Anisotropy of its Reaction with Ammonia Gas
Journal of American Chemical Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Rodger S. Miller, David Y. Curtin, and Iain C. Paul
Reactions of Molecular Crystals with Gases III. The Relationship of Anisotropy to Crystal Structure in Reactions of Carboxylic Acids and Anhydrides with Ammonia Gas
Journal of American Chemical Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Iain C. Paul and David Y. Curtin
Reactions of Organic Crystals with Gases
Science (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GP-34545X

David A. Dieterich, Iain C. Paul, and David Y. Curtin
Structural Studies on Nitrosobenzene and 2-Nitrosobenzoic Acid. Crystal and Molecular Structures of cis-Azobenzene Dioxide and trans-2,2'-Dicarboxyazobenzene Dioxide
Journal of American Chemical Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract HC-15-67-0221, and by the National Science Foundation Fellowship

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Arnold Reed Miller (David Curtin, Adviser)
Rotationally-Locked cis-Diarylacenaphthenes: Syntheses and Proton Magnetic Resonance Studies
September 1973
(Not MRL supported)

Electron-Phonon Interactions in Simple Metals

Principal Investigator: John Dow, Ph.D.
Associate Professor of Physics

Supporting Agency: National Science Foundation

Senior Staff: John Dow, Professor
Donald Franceschetti, Research Associate

Junior Staff: Marshall Bowen, Research Assistant
Jess F Fauchier, Research Assistant (Term 3/8/74)
Darryl Smith, Research Assistant

Objectives: The long-range objective of this theoretical research program is to understand the electronic properties of real solids in local (r-space) framework. En route to this goal we have studied the effects of localized core holes on soft x-ray spectra of solids and we have attempted to better understand electron-phonon interactions and their effects on the transport properties of simple metals.

Approach: Available theoretical techniques have been used to solve problems of experimental and theoretical importance.

In the case of x-ray spectra, we have derived numerous sum rules and constraints on data which follow from many-electron theory and general principles of physics. Analyses of data using these general results have pointed out the paths to new theories.

Present work centers on theories of electron-energy loss spectra, which provide sensitive tests of many-electron theories.

In the case of the transport properties of simple metals, a new theory of thermoelectric effects has been developed, and computations of the thermopowers of the alkali metals of Li, Na, and K executed.

Progress: (01 07 73 - 30 06 74) The existing theory of x-ray edges has been demonstrated to be incomplete, and it has been shown that no experimental evidence for Anderson orthogonality catastrophes exists in x-ray data (as once thought). We are presently developing alternate theories of x-ray spectra, which should satisfy the sum rules derived earlier.

It has been shown that (contrary to widespread opinion) for Li, Na, and K the thermoelectric powers are less sensitive to input parameters such as pseudopotentials, then the resistivities. The resistivities, Hall coefficients, and thermopowers of these materials have been successfully computed as functions of pressure. A new formal expression for thermopowers has been developed and demonstrates the combined importance of anisotropy and energy dependent-scattering for finding metals with large themoelectric powers.

In addition, studies of strong-field Stark effects, catalysis of $C_2H_6+H_2 \rightarrow 2CH_4$, and large many-electron enhancement of Auger rates have been successfully pursued.

Publications: (01 07 73 - 30 06 74)

John D. Dow
Effects of Final-state Interactions on Modulation
Spectra of Semiconductors
Surface Science 37, 786-803 (1973)
Supported by the National Science Foundation under Grant GH-33634

John D. Dow, Darryl Lyle Smith, and Frank L. Lederman
Acceptor-to-Band Transitions in Semiconductors: Photoluminescence,
Exponential Absorption Edges, and Final-State Interactions
Physical Review B8, 4612-4626 (1973)
Supported by the National Science Foundation under Grant GH-33634

John D. Dow
Screening-enhanced Optical Absorption and the Search for M_3 Critical-points
Physical Review Letters 30, 903-906 (1973)
Supported by the National Science Foundation under Grant GH-33634

Jess Fauchier and John D. Dow
An Analytic Approach to the Hydrogen Stark Effect in Weak, Strong, and Ultra-strong Fields
Physical Review A9, 98-107 (1973)
Supported by the National Science Foundation under Grant GH-33634

John D. Dow
Compatibility Relationships for X-ray Threshold Shapes
Physical Review Letters 31, 1132-1135 (1973)
Supported by the National Science Foundation under Grant GH-33634

John D. Dow, John E. Robinson, and Thomas R. Carver
The Mahan Soft X-ray Anomaly in Lithium: Relationship to the Knight Shift
Physical Review Letters 31, 759-762 (1973)
Supported by the National Science Foundation under Grant GH-33634, AFOSR (Illinois), by the Atomic Energy Commission (Argonne), and by NSF (Princeton)

John D. Dow and Bernd F. Sonntag
X-ray Edges of Simple Metals: Dependence on Electron Density
Physical Review Letters 31, 1461-1463 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132

D. L. Smith and John D. Dow
Divergent Enhancement of Forbidden X-ray Edges by Lattice Vibrations
Physical Review B9, 2509-2512 (1974)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132

John D. Dow and D. L. Smith
The Role of the Cut-off Energy in Tests of the X-ray Threshold Theory
physica status solidi (b) 63, (1974)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132

John D. Dow and Darryl Lyle Smith
X-ray Spectra of Metallic Alloys: Many-Electron Effects
Journal of Physics F: Metal Physics (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132

John D. Dow
K-edge X-ray Spectra of Mg and Other Simple Metals; The Absence of Evidence for Orthogonality Catastrophes
Physical Review (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132

John D. Dow, John E. Robinson, John H. Slowik, and Bernd F. Sonntag
On the Theory of Soft X-ray Absorption Thresholds: Amorphous Mg_xSb_{1-x} Alloys and Metallic Li, Na, Mg, and Al
Physical Review (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132, by U. S. Army Research Office (Durham), and by the Advanced Research Projects Agency under Contract HC-15-67-C-0021

John D. Dow, John E. Robinson, and Thomas R. Carver
Theories of X-ray Edge Anomalies
Physical Review (submitted to)
Supported by the National Science Foundation under Grants GH-33634, GH-39132, and GP-19891

Donald R. Franceschetti and John D. Dow
Auger Rates for Soft X-ray Transitions in Ionic, Atomic, and Metallic Lithium
Journal of Physics F (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132

John D. Dow, Lewis N. Watson, and Derek J. Fabian
On the K X-ray Emission Edge-shapes of Free-electron Metals
Journal of Physics F (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132

John D. Dow, Darryl L. Smith, and Bernd F. Sonntag
X-ray Spectra of Aluminum
Physical Review (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-39132, and by U. S. Army Research Office (Durham) D31-124-71-G103

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Jess F. Fauchier II (John D. Dow, Adviser)
Topics in the Theory of Condensed Matter: Electron Field Emission, Field Ionization, and Ethane Catalysis
June 1974
Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, and by AFOSR

Mass Spectroscopy, Spectrochemistry Research

Principal Investigator: Charles A. Evans, Jr., Ph.D.
Senior Research Chemist

Supporting Agency: National Science Foundation

Senior Staff: Charles A. Evans, Jr., Senior Research Chemist
Bruce N. Colby, Research Chemist (Term 2/1/74)
David S. Simons, Research Associate

Objectives: The objectives of this program are to study the basic phenomena involved in analytical spectroscopy and to develop improved instrumentation and analytical techniques for the characterization of materials. This research is primarily directed to mass spectrometric techniques.

Approach: Two major areas of investigations are currently underway in the study of spectroscopic processes. The first involves the study of electrohydrodynamic (EH) ionization for direct ion production from a liquid surface for mass spectrometric analysis. The research during FY74 has studied the organic liquid, glycerol, containing dissolved non-volatile organic compounds. The second area is primarily in the study development and analytical applications of ion microprobe mass spectrometry with some activity in the more general areas of microchemical and surface characterization.

Progress: (01 07 73 - 30 06 74) Operation of the EH ion source on a liquid organic, glycerol, (Gly) has been accomplished by using a salt (NaI, KCl, and $SnCl_3$) doping of the glycerol to render it conducting. The resultant mass spectra contain two polymeric ion types; $H(Gly)_n^+$ and $Na(Gly)_n^+$. The latter is exemplary of the ion composition when NaI doping is used.

Two thermally labile compounds, proline (an amino-acid) and sucrose (a carbohydrate), have been added to the glycerol, subjected to EH ionization and mass spectra obtained. The proline and sucrose produced a polymeric ion series similar to the glycerol as well as ions resulting from combinations of proline and glycerol and sucrose and glycerol. Fragment ions comprised less than one percent of the total ion yield. These results demonstrate that the EH ionization process can produce ions of non-volatile, thermally labile organic compounds and may be useful as a method for probing liquid state or field induced liquid state reactions.

The secondary ion mass spectrometry (SIMS) research has involved two areas of investigation during FY74. The first has been the development and evaluation of a large beam ion probe attachment for the MS-7 presently in the Materials Research Laboratory. This device can be quickly attached to and removed from the mass spectrometer, provides for surface analysis and thin film profiling in both the electrical and photographic detection modes (under either high and low mass resolution conditions) and can provide an ion probe capability when a laboratory does not have the need or resources for a complete ion microprobe system. The second area of SIMS research has dealt with instrumentation and analytical techniques for the ion microprobe mass spectrometer. The instrumentation aspects of this research have dealt mainly with the production of the primary ions and the extraction of the secondaries into the mass spectrometer. Modifications to the duoplasmatron primary ion source have increased the positive ion current density at the

sample surface by approximately one order of magnitude and provided for the negative ion bombardment of the sample. This latter feature is specifically required for the analysis of insulators. As a result of this instrumental improvement and our high mass resolution ion microprobe research we have begun the study of complex, insulating matrices such as glasses and teeth.

Other research progress during FY74 resulted in the development of a hollow-cathode ion source for the mass spectrometry of solids and provided very valuable information on the toxic element concentration vs. particle size distribution for airborne particles emitted from a coal-fired power plant. The hollow-cathode ion source emission is dc making it very amenable to electrical detection techniques, it produces few interfering doubly-charged or molecular ions, it has relatively uniform excitation from element to element, and it seems to have sub-ppm detection limits. From our preliminary evaluation the hollow cathode source has the potential to be a valuable ion source for the mass spectrometry of solids.

The study of airborne particulates has been a cooperative study with Professor D. F. S. Natusch of the Department of Chemistry. This work has shown that the toxic trace elements are preferentially concentrated in the smallest particles. A surface condensation or adsorption mechanism has been postulated as the reason for higher concentrations in those particles with a high surface to volume (or weight) ratio. The environmental significance lies in the fact it is these small particles which most easily evade present emission control devices and most readily interact with the human body via

inhalation and dissolution in the lung. This study is being continued to confirm the surface adsorption mechanism and to provide information relevant to improving emission control processes.

Publications (01 07 73 - 30 06 74)

C. A. Evans, Jr.
Ion Probe Mass Spectrometry: Overview
Thin Solid Films 19, 11-19 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-33273

D.F.S. Natusch, J. R. Wallace, and C. A. Evans, Jr.
Toxic Trace Elements: Preferential Concentration in Respirable Particles
Science 183, 202-204 (1974)
Supported by the National Science Foundation under Grants GH-33634 and GI-31605

D. K. Bakale, B. N. Colby, C. A. Evans, Jr., and J. B. Woodhouse
Reduction of Spectral Interferences in Ion Probe Mass Spectrometry
Proceedings of the 8th National Meeting of the Electron Probe Analysis Society of America, New Orleans, pp. 7A-7D (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-33273 and by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

C. A. Evans, Jr.
Secondary Ion Mass Spectrometry - The Ion Probe
Proceedings of the Tutorial Session of the 8th National Meeting of the Electron Probe Analysis Society of America, New Orleans, pp. 29-72 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-33273

D. Natusch, R. Davison, R. E. Lamb, J. R. Wallace, and C. A. Evans, Jr.
Trace Metals in Airborne Particles
Proceedings of the Third Clean Air Congress, Dusseldorf, C12-14 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GI-31605

B. N. Colby and C. A. Evans, Jr.
Hollow-Cathode Ionization for the Mass Spectrometric Analysis of Conducting Solids
Analytical Chemistry (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Richard L. Davison, David F. S. Natusch, John R. Wallace, and C. A. Evans, Jr.
Trace Metals in Fly Ash: Dependence of Concentration on Particle Size
Environmental Science and Technology (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GI-31605-IES-7

W. K. Chu, M-A. Nicolet, J. W. Mayer, and C. A. Evans, Jr.
Comparison of Backscattering Spectrometry and SIMS Analysis of Ta_2O_5 Layers
Analytical Chemistry (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GP-33273, and by the Office of Naval Research (L. Cooper)

R. J. Blattner, J. E. Baker, and C. A. Evans, Jr.
A Simple Ion Probe Attachment for Existing Mass Spectrometers
Analytical Chemistry (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GP-33273

D. K. Bakale, B. N. Colby, and C. A. Evans, Jr.
High Mass Resolution Ion Microprobe Mass Spectrometry of Complex Matrices
Analytical Chemistry (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GP-33273

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Electronic Structure of Metallic Alloys

Principal Investigator: Colin P. Flynn, Ph.D.
Professor of Physics

Supporting Agency: National Science Foundation

Senior Staff: Colin P. Flynn, Professor
Alfred A. Fote, Research Associate (Term 1/31/74)
E. E. Pollock, IBM Postdoc Fellow

Junior Staff: R. Phillip Layton, Research Assistant
Daniel J. Phelps, Research Assistant
Richard A. Tilton II, Research Assistant

Objectives: The aim of this project is to improve the present misunderstanding of the bulk and surface properties of materials. The recent focus has been on local ground and excited configuration of impurity atoms in metals and on clean metal surfaces, and on their migratory behavior.

Approach: Excited configurations of impurity atoms interacting with bulk metals and with clean metal surfaces are under investigation by optical techniques, including vacuum ultraviolet absorption spectroscopy and magneto optic measurements, and by transport measurements. Concurrent theoretical studies elucidate the observations in terms of impurity structure. Both quantum mechanical and classical molecular dynamical methods are being applied to kinetic problems associated with atomic motion in bulk materials and to those surface processes relevent to catalysis.

Progress: (01 07 73 - 30 06 74) The optical excitation spectra of rare gas impurities in metallic hosts have been comprehensively studied and interpreted. The excitation threshold is sharp and may be predicted by theory quite accurately. The absorption above threshold shows that only

a single excited quasiparticle accompanies the optical excitation near threshold in p→s transitions. This precise result cannot be reconciled with existing theories, and it appears that widely accepted Hartree-Fock theories fail to describe these optical processes with reasonable fidelity. Sharp pair spectra associated with pairs of rare gas atoms in metallic hosts have been discovered and their unique width explained. The excited configurations both for like and unlike rare gas pair combinations contain virtual levels associated with "united atom" states of the diatomic rare gas molecule, and this explains the lack of broadening that arises in other cases from concurrent electron-hole pair creation. Work is now shifting to studies of other impurity types such as halogen, 3d and 4f impurities in metals. There are in progress studies of hydrogen in metals under ONR funding. In related work a magneto optic apparatus, for use in the same energy range, has been constructed and is almost fully tested. It will be used to analyze local ground state susceptibilities and excited configuration spin-orbit couplings associated with impurities in metals. Apparatus for use in similar proposed studies of surface atoms now approaches completion, but progress has been delayed by a temporary lack of staff.

In a second area, also related to catalysis and chemisorption, molecular dynamics programs are being developed for detailed studies, using the Illiac 4 computer, of the motion of migrating atoms on surfaces and in the bulk. Simulation of the interaction between molecular systems and metal surfaces is one aspect of this work. Concurrent quantum mechanical studies of light particle motion are in progress.

Publications: (01 07 73 - 30 06 74)

C. P. Flynn and J. A. Rigert
Impurity Diamagnetism in Metals
Physical Review B7, 3656-3671 (1973)
Supported by the National Science Foundation under Grant GH-33634
and by the Advanced Research Projects Agency

C. P. Flynn
Configurational Energies of High-Valence Impurities Dissolved in Metals
Physical Review B4, 1984-1986 (1974)
Supported by the National Science Foundation under Grant GH-33634

C. P. Flynn
Effect of Electronic Correlations in the X-ray Edge and Recoil Problems
Physical Review Letters 32, 1058 (1974)
Supported by the National Science Foundation under Grant GH-33634

R. A. Tilton, D. J. Phelps, and C. P. Flynn
Optical Absorption Threshold in Dilute Alkali Metal-Rare Gas Alloys
Physical Review Letters 32, 1006 (1974)
Supported by the National Science Foundation under Grant GH-33634

C. P. Flynn
Magnetic Effects of Charge Transfer
Proceedings of AIME Meeting, Philadelphia 1973 (to be published)
Supported by the National Science Foundation under Grant GH-33634

C. P. Flynn
Charge Transfer Complexes in Metals
Solid State Physics (submitted to)
Supported by the National Science Foundation under Grant GH-33634

E. N. Koch and C. P. Flynn
Sharp Coupling Transition of Gd in AlGa Alloys
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Experimental Studies of Superconductors

Principal Investigator: Donald M. Ginsberg, Ph.D.
Professor of Physics

Supporting Agency: National Science Foundation

Senior Staff: Donald M. Ginsberg, Professor
Patrick Tai, Research Associate

Objectives: To test experimentally the theory of Rusinov, Shiba, Nagi, and others of the interactions of electrons in superconductors with strongly perturbing magnetic impurities. The research is of fundamental importance, and is also relevant to the development of thin-film superconducting devices.

Approach: Precision measurements of the specific heat of superconducting film samples. An ac specific heat technique is to be used. The film is flash-evaporated to avoid precipitation of the impurities.

Progress: (01 07 73 - 30 06 74) We have designed modifications of an all-metal cryostat for our flash evaporations and specific heat measurements, and we are now putting the equipment into operation.

In another investigation, we have completed measurements of the thermal conductivity of thin superconducting indium films in contact with normal or superconducting thallium films. The results agree well with a theoretical model which we created. This lends support to the present theory of inhomogeneous superconductors.

We have performed two computer calculations to determine physical parameters. One determined from first principles for the first time the

temperature dependence of the electromagnetic coherence length of superconductors (Pb and $Pb_{0.9}Bi_{0.1}$) in which the electron-phonon coupling is sufficiently strong to introduce structure in the dependence of the gap parameter as a function of energy. The other calculation yielded the electromagnetic surface resistance of a superconducting aluminum alloy. It provided a definitive check on the theory of electromagnetic absorption in superconductors. The results agree with the previously published experimental data.

Publications: (01 07 73 - 30 06 74)

B. J. Mrstik and D. M. Ginsberg
Electron Thermal Conductivity of Superconducting Films of Indium-Gadolinium and Lead-Gadolinium Alloys
Physical Review B7, 4844-4850 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-28996

D. M. Ginsberg
The Electromagnetic Surface Resistance of a Superconducting Aluminum Alloy
Physical Review B8, 2358-2359 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-28996

H. R. Kerchner and D. M. Ginsberg
Temperature Dependence and Low-Temperature Value of the Electromagnetic Coherence Length in Superconducting Pb and $Pb_{0.9}Bi_{0.1}$
Physical Review B8, 3190-3193 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-28996

A. Migliori and D. M. Ginsberg
Influence of the Proximity Effect on the Electron Thermal Conductivity of Superconducting Thin-Film Sandwiches of Indium and Thallium
Physical Review B8, 5065-5071 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GH-37980

D. M. Ginsberg
The Depression of the Superconducting Transition Temperature Caused by Iron-Group Magnetic Impurities
Physical Review (Comments and Addenda) (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-37980

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Albert Migliori (D. M. Ginsberg, Adviser)
Electron Thermal Conductivity of Thin Superconducting Films in Metallic Contact - The Proximity Effect
October 1973
Supported by the National Science Foundation under Grants GH-33634 and GP-28996

Optical Properties of Solids

Principal Investigator: Paul Handler, Ph.D.
Professor of Physics and Electrical Engineering

Supporting Agency: National Science Foundation

Senior Staff: Paul Handler, Professor

Objectives: To determine the band structure of solids and the properties of surfaces and interfaces to provide basic information for choice of materials for electronic devices.

Approach: Measurement of electroreflectance spectra of semiconductors and ferroelectrics.

Progress: (01 07 73 - 30 06 74) During this period the project is being terminated due to a change in staff interest. A paper reporting on work done previously is listed below.

Publications: (01 07 73 - 30 06 74)

Stephan A. Mack and Paul Handler
Electroreflectance of Strontium Titanate
Surface Science 37, 280-287 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Army Research Office

Joel W. Grover and P. Handler
Electroreflectance of Silicon
Physical Review B9, 2600-2606 (1974)
Supported by the National Science Foundation under Grant GH-33634

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Mechanical and Thermal Properties of Solids

Principal Investigator: Jon T. Holder, Ph.D.
Assistant Professor of Geology

Supporting Agency: National Science Foundation

Senior Staff: Jon T. Holder, Assistant Professor

Junior Staff: David M. Joncich, Teaching Assistant
Sekyung Lee, Research Assistant
Lynn E. Rehn, Research Assistant (Term 12/17/73)
Richard J. Wallat, Research Assistant

Objectives: An understanding of mechanical and thermal properties that are of interest to solid state physics and geophysics. Principal areas of interest are: 1) elastic properties of perfect crystals and its use in calculating thermal properties; 2) the mechanical behavior of materials containing defects, especially dislocations.

Approach: The study of a particular material using a variety of types of measurements. This approach is based on the fact that simultaneous measurements on a single specimen often provide more than a proportionate amount of information. In the investigation of the mechanical properties of ice, ultrasonic, sonic, microstrain, static stress, and dielectric techniques are used. The response of dislocations to cyclic low frequency stresses and electric fields in the 0.01 - 100 Hz range is used to determine the microscopic motions of the dislocations, and hence the mechanisms limiting plastic flow, in ice. Macroscopic plastic behavior is also monitored with the static stress techniques. In the study of structural phase transformations in alkali halides ultrasonic velocity measurements are being carried out

while simultaneously applying hydrostatic and uniaxial stresses. The results will be compared to the atomistic calculations of the transformation energies in order to investigate the extent to which elasticity considerations can be used to predict transformation properties (such as the effects of non-hydrostatic stresses).

Progress: (01 07 73 - 30 06 74) The analysis of the effects of slow neutron irradiation in elastic constants of copper has been completed. The investigation provided the first experimental evidence for: the <100> split configuration for free interstitials; the existence of theoretically predicted low frequency resonant modes of oscillation of interstitials; and a model for one of the close pair configurations in copper.

Calculations of analytic expressions of the Gibbs energy of alkali halides as a continuous function of a single deformation parameter during the transformation from the NaCl to the CsCl structure have been carried out. The expressions calculation has been checked by comparison with numerous existing measurements of transformation properties in rubidium halides, and the third order constants of RbCl have been measured and also found to agree with the calculated results.

Dislocation motions in ice, undetectable in previous MHz, KHz, and 100 Hz measurements, have been observed with microstrain measurements in the .01 - 10 Hz range. Preliminary measurements indicate that microscopic and macroscopic dislocation motions can be separated, facilitating the study of the mechanisms which determine plastic flow in ice.

Publications: (01 07 73 - 30 06 74)

J. Holder, A. V. Granato, and L. E. Rehn
Experimental Evidence for Split Interstitials in Copper
Physical Review Letters (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and
by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

L. E. Rehn, J. Holder, A. V. Granato, R. R. Coltman, F. W. Young, Jr.
Effects of Thermal Neutron Irradiation on the Elastic Constants of Copper
Physical Review Letters (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and
by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

J. Holder, A. V. Granato, and L. E. Rehn
Effects of Interstitials and Close Pairs on Elastic Constants
Physical Review Letters (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and
by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Lynn Eduard Rehn (J. Holder, Adviser)
Contributions from Point Defects to the Elastic Constants of Copper
February 1974
Supported by the National Science Foundation under Grant GH-33634 and
by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Electronic Structure of Solids

Principal Investigator: A. Barry Kunz, Ph.D.
Associate Professor of Physics

Supporting Agency: National Science Foundation

Senior Staff: A. Barry Kunz, Associate Professor

Junior Staff: Michael P. Guse, Research Assistant
Kent M. Hall, Research Assistant

Objectives: The overriding objective of this research has been to develop ab initio method for studies of electronic properties of solids which are reliable, accurate and efficient of both human and computer resources. The secondary objective has been to take the techniques developed and to apply them to studies of the physical properties of real solids.

Approach: The fundamental approach of all these studies undertaken has been similar. The first step is solving the Hartree-Fock problem via the intermediary of the local orbitals transformation (this results in efficiency). The second state has been to develop techniques whereby effects of correlation and relaxation may be incorporated in the calculation (a variety of methods are developed and used). It is quite important to correlate Hartree-Fock energy bands in our opinion. Without correlation the Fock band gaps in insulators are too wide by 4 - 8 eV and the state density at the Fermi energy of a metal is zero. Correlation has been shown to eliminate these defects properly. In some studies we assume the solid to be infinite and three dimensional and in others we have studied molecular fragments (clusters)

of the solid. This latter approach is of some use in studying chemical properties, whereas the former is useful for studying the electronic structure of the solid.

Progress: (01 07 73 - 30 06 74) The major achievements of the past year in this research have been threefold.

(1) We have generated a successful, efficient, compact computer code for studying the electronic structure of simple solids (cubic lattice and one or two atoms per Wigner-Seitz cell). This code has been applied to studying solids as diverse as Ar, LiH, and Ca. One substantial benefit of the calcium study was an ability to predict accurately the change of calcium from a metal to a semi-metal and back to a metal as one applied hydrostatic pressure to the solid.

(2) We have generated a set of theories, ideas, and computer codes to permit us to include correlation-relaxation effects on the electronic structure of solids. The range of applicability of our methods developed ranges from metals to insulators.

(3) We have developed a theory of soft x-ray interaction in solids which makes clear the fundamental distinction between optical absorption experiments and photoemission ones. We predict a breakdown of the one-electron quasi particle description of occupied levels. This says that apparent splitting between two occupied states will depend upon the measurement. The degree of splitting will be ~ 0.5 eV for a non-polar material to ~ 10.0 eV for some pairs of levels in polar materials.

Publications: (01 07 73 - 30 06 74)

P. W. Deutsch and A. Barry Kunz
Core Excitation Spectra for CH_4 and SiH_4
Journal of Chemical Physics 59, 1155-1158 (1973)
Supported by the National Science Foundation under Grant GH-33634

A. Barry Kunz
Systematic Extension of the Local-Orbitals Method
Physical Review B7, 5369-5379 (1973)
Supported by the National Science Foundation under Grant GH-33634
and by the Aerospace Research Lab F33615-72-C-1506

Daniel J. Mickish and A. Barry Kunz
Energy Bands in LiF and Solid Ar
Journal of Physics 6, 1723-1733 (1973)
Supported by the National Science Foundation under Grant GH-33634, by
U. S. Army Research Office DAHC-04-69-C0007, and by the Aerospace
Research Lab F33615-72-C-1506

A. B. Kunz and D. J. Mickish
Energy Bands in LiH
Journal of Physics C: Solid State 6, 83-85 (1973)
Supported by the National Science Foundation under Grant GH-33634, by
U. S. Army Research Office DAHC-04-69-C0007, and by the Aerospace
Research Lab F33615-72-C-1506

A. B. Kunz, D. J. Mickish, and P. W. Deutsch
On the Interaction of a Hydrogen Atom with a Lithium Metal Surface
Solid State Communications 13, 35-38 (1973)
Supported by the National Science Foundation under Grant GH-33634,
by the U. S. Army Research Office under Contract DA-HC04-69-C0007,
and by the Aerospace Research Lab under Contract F33615-72-C-1506

A. Barry Kunz and Daniel J. Mickish
A Study of the Electronic Structure and the Optical Properties of the
Solid Rare Gases
Physical Review B8, 779-794 (1973)
Supported by the National Science Foundation under Grant GH-33634,
by the U. S. Army Research Office under Contract DA-HC04-69-C0007,
and by the Aerospace Research Lab under Contract F33615-72-C-1506

A. Barry Kunz
A Simplified Hartree-Fock Method for Calculating Ground State Properties
and Energy Band Structures
Physical Review B8, 1690-1698 (1973)
Supported by the National Science Foundation under Grant GH-33634,
and by the Aerospace Research Lab

A. Barry Kunz, Daniel J. Mickish, and Thomas C. Collins
Absorption of Soft X-ray by Insulators with a Forbidden Exciton Transition
Physical Review Letters 31, 756-759 (1973)
Supported by the National Science Foundation under Grant GH-33634, by the Aerospace Research Lab under Contract F33615-72-C-1506, and by the U. S. Army Research Office under Contract DA-HC04-69-C0007

A. Barry Kunz and T. C. Collins
Development of Non-Local One Particle Excitation Hamiltonian for Atomic, Molecular, and Solid State Systems
Journal of Physics B7, L69-L72 (1974)
Supported by the National Science Foundation under Grant GH-33634 and by the Aerospace Research Lab under Contract F33615-72-C-1506

T. C. Collins, A. B. Kunz, and J. T. Devreese
An Excited State of Alkali Halides
International Journal of Quantum Chemistry Symposium 7, 551-557 (1973)
Supported by the NATO Research Grant No. 509, by the Advanced Research Projects Agency under Contract HC15-67-C-0221, and by the Aerospace Research Lab under Contract 33-615-72-C-1506

T. C. Collins and A. B. Kunz
Calculation of Excitation Energies of Atomic Systems Using $\hat{O}\hat{A}\hat{O}$
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

P. W. Deutsch and A. Barry Kunz
Computation of Some Optically Allowed Soft X-ray Transitions in Molecular CH_4 and Neon
Journal of Chemical Physics (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Daniel J. Mickish, A. Barry Kunz, and T. C. Collins
Optical Properties of LiF
Physical Review B (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Sokrates T. Pantelides, Daniel J. Mickish, and A. Barry Kunz
Correlation Effects in Energy-Band Theory
Physical Review (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and NSF-39811

Sokrates T. Pantelides
Theory for the Binding Energies of the First-Row, Deep Donors in GaP and Si
Physical Review Letters (submitted to)
Supported by the National Science Foundation under Grants GH-33634 (Illinois) and GH-39811 (Stanford), and by the Aerospace Research Lab under Contract F33615-72-C-1506

J. C. Campbell, N. Holonyak, Jr., A. B. Kunz, and M. G. Craford
Model Calculations for Radiative Recombination in Zn-N-Doped $GaAs_{1-x}P_x$ in the Direct and Indirect Composition Region
Physical Review (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-33771, and by the Aerospace Research Laboratory

J. C. Campbell, N. Holonyak, Jr., A. B. Kunz, and M. G. Craford
Effect of Crystal Composition on "Quasi-Direct" Recombination and LED Performance in the Indirect Region of $GaAs_{1-x}P_x$:N
Journal of Applied Physics Letters (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-33771, and by the Aerospace Research Laboratory

A. Barry Kunz
Distinction Between Optical Absorption Edges and Photo-Emission Edges in Solids
Journal of Physics (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Aerospace Research Lab under Contract F33615-72-C-1506

Sokrates T. Pantelides, Daniel J. Mickish, and A. Barry Kunz
An AB INITIO Study of the Electronic Properties of Magnesium Oxide
Solid State Communications (submitted to)
Supported by the National Science Foundation under Grant GH-33634, by the Aerospace Research Lab under Contract F33615-72-C-1506, and by the U. S. Army Research Office under Contract DAHC-04-69-C0007

T. C. Collins, D. Esterling, D. J. Mickish, and A. Barry Kunz
Comments on the Energy Band Structures of the Solid Rare Gas Mixtures
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Aerospace Research Lab under Contract F33615-72-C-1506

V. E. Van Doren and A. Barry Kunz
Approximate Calculation of the Electronic Structure of Solid Surfaces and Interfaces Between Material Media
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Aerospace Research Lab under Contract F33615-72-C-1506

A. Barry Kunz
Optical Absorption and Photo Emission Edges in Insulating Solids
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Aerospace Research Lab under Contract F33615-72-C-1506

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Peter Wehner Deutsch (A. Barry Kunz, Adviser)
Optical Properties of Simple Molecules
October 1973
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

Thermodynamic Properties of Materials

Principal Investigator: Dillon E. Mapother, D.Sc.
Professor of Physics,
Director, Computing Services Office

Supporting Agency: National Science Foundation

Senior Staff: Dillon E. Mapother, Professor
Elemer Papp, Research Assistant Professor

Objectives: High resolution methods are used to study the temperature dependence of the specific heat of magnetic materials near Curie point anomalies. The effect of increasing concentrations of copper on the shape and critical temperature of nickel is being investigated.

Approach: Phase sensitive detection is used to measure temperature oscillations in a small specimen exposed to pulsed light. Dilute alloys of copper in nickel are prepared by high temperature diffusion of copper vapor into pure single crystal specimens of nickel.

Progress: (01 07 73 - 30 06 74) Effect of Alloying on the Specific Heat Anomaly at the Curie Point of Nickel. Substantial improvements in the quality of the specific heat measurements have been verified. These improvements result partly from changes in the details of the measuring technique and partly from improved procedures of specimen preparation. Details will be reported separately.

Measurements of the specific heat transition have been completed for a series of single crystalline alloys of Cu in Ni covering the concentration range from 0-10% Cu. Sharp transitions are observed up to 5% Cu concentration, above which a noticeable broadening effect becomes evident.

The data are now being analyzed to show the effect of alloy concentration on the various critical parameters of the Curie point transition. A preliminary report is being prepared for publication.

Measurements of specific heat and thermoelectric power have also been made in the same Ni specimen. These observations are of interest in establishing the correspondence between separate physical manifestations of the Curie point transition. Analysis of these data is incomplete at this writing.

Publications: (01 07 73 - 30 06 74)

None

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Investigations of Cooperative Phenomena at Low Temperatures

Principal Investigator: Jack M. Mochel, Ph.D.
Associate Professor of Physics

Supporting Agency: National Science Foundation

Senior Staff: Jack M. Mochel, Associate Professor

Junior Staff: Edward L. Griffin, Research Assistant
Daniel L. Rascoe, Research Assistant
James E. Rutledge, Research Assistant
Lawrence N. Smith, Research Assistant

Objectives: An understanding of the thermodynamics of surfaces and of the effect of thermal fluctuations in real two and three dimensional systems.

Approach: To study He^4 in its two dimensional, superfluid state we have created a "two dimensional" resonant cavity. The desired amount of helium gas is diffused through the walls of a quartz capsule at room temperatures. At low temperatures this gas coats the inner surface of the capsule with a superfluid film a few atomic layers thick. This closed surface supports third sound waves. Since this capsule can be reused, accurate studies of Van der Waals force, superfluidity and thermodynamic fluctuations can be made. Using the same capsule, measured amounts of He^3 can also be added. Below 1°K, He^3 will float on the He^4 film. We have also placed capacitor plates within the walls of this capsule to monitor pressure.

Using an ac heat capacity technique where we have achieved a resolution of 10^{-11} j/K° we are able to observe the effect of thermodynamic fluctuations in two dimensional systems. The traditional method of measuring

the heat capacity at these temperatures may only achieve a resolution of 10^{-5}j/deg. We are further increasing the resolution by using a thin film thermometer and interfacing a computer to eliminate long term drift.

Monochromatic phonons are being generated with a double, superconducting tunnel junction and with ESR at 70 GHz in CaF_2. These phonons will be used to study the behavior of bulk helium and surfaces at low temperatures.

Progress: (01 07 73 - 30 06 74) We are now carrying out third sound measurements down to 30 mK. He^3 has a profound effect on the surface of our films and we expect to observe the two dimensional transition of He^3 surface states. In addition we are now able to also measure pressure with a resolution of better than 10^{-3}Torr. Because of the small size of our system this pressure corresponds to the excitations of the He^3 surface states.

We have developed a secondary thermometer of small mass to improve our ac heat capacity measurements of superconductors and liquid crystals. This thermometer is a 20 Å thick film of CuNi sandwiched between layers of SiO. Although, because of its thinness, it has a shelf-life of only a month, it also has several virtues. The range of useful temperature can be set from 0.1 K up to 100 K. The calibration is stable to better than 0.5 mK/2 days, it is independent of magnetic field up to at least 25 Kg and its total thickness, including SiO is only 1500 Å. Such thermometers are of use not only because of their small size or insensitivity to magnetic field but also they are able to measure temperature within atomic distances of a surface.

Publications: (01 07 73 - 30 06 74)

J. E. Rutledge, T. E. Washburn, and J. M. Mochel
Shielded Cable for Use in Low-Temperature Experiments
Review of Scientific Instruments (Notes) 45, 135 (1974)
Supported by the National Science Foundation under Grant GH-33634

E. L. Griffin and J. M. Mochel
Thin Low Temperature Metal Film Thermometers
Review of Scientific Instruments (submitted to)
Supported by the National Science Foundation under Grant GH-33634

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Properties of Magnetic Materials

Principal Investigator: Myron B. Salamon, Ph.D.
Associate Professor of Physics

Supporting Agency: National Science Foundation

Senior Staff: Myron B. Salamon, Associate Professor
Robert A. Craven, Research Associate

Junior Staff: Ray M. Herman, Research Assistant
William Miniscalco, Research Assistant
Mark J. Schaffman, Research Assistant

Objectives: The experimental investigation of physical properties near phase transitions, especially magnetic and structural transitions. Of particular interest are the roles of lattice dimensionality, symmetry of the ground state, and the number of spin degrees of freedom on the properties of the phase transition. The nature of the metal insulator transition in quasi- one-dimensional organic salts and of the exciton-to-electron-hole liquid transition in Ge are also being studied.

Approach: Thermodynamic (specific heat and thermal diffusivity) measurements, electronic and nuclear spin resonance, and measurements of the electrical resistivity are made in the vicinity of phase transitions. Usually more than one measurement is made on a particular sample in order to exploit theoretical relationships between the various properties. Extensive use is made of the computer in analysis of critical point data. The electron-hole liquid will be studied through light scattering and luminescence.

Progress: (01 07 73 - 30 06 74) 1. The specific heat and thermal diffusivity of the conducting salt tetrathiofulvalinium-tetracynoquinodimethane (TTF-TCNQ)

have been measured on the same samples and have been combined to give the thermal conductivity. An anomaly in the specific heat at the metal insulator transition has been found and a decrease in the thermal conductivity at the same temperature. These have been interpreted in light of models for the metal-insulator transition.

2. Electron-spin resonance measurements have been made on TTF-TCNQ and preliminary studies of the microwave conductivity begun using a bimodal microwave cavity.

3. The "universality hypothesis" of critical behavior has been tested for both Heisenberg- and Ising-like phase transitions and found to hold for a wide variety of materials. Data from our own measurements and from the literature were analyzed in a novel manner which brought the disparate values of the critical exponents of the specific heat into agreement.

4. A spectrometer has been constructed and the luminescence from excitons and the electron-hole liquid phases of Ge has been observed. Measurement of the coexistence curve of the two phases is underway.

Publications: (01 07 73 - 30 06 74)

M. B. Salamon and P. M. Richards
EPR in K_2MnF_4: A two-dimensional Heisenberg Paramagnet
Proceedings of the AIP Conference on Magnetism and Magnetic Materials
pp. 187-191 (1973)
Supported by the National Science Foundation under Grant GH-33634

Guenter Ahlers, Avinoam Kornblit, and Myron B. Salamon
Heat Capacity of FeF_2 Near the Antiferromagnetic Transition
Physical Review B9 (1974)
Supported by the National Science Foundation under Grant GH-33634

R. A. Craven, M. B. Salamon, G. DePasquali, R. M. Herman, G. Stucky, and A. Schultz
The Specific Heat of Tetrathiofulvalinium-Tetracyanoquinodimethane in the Vicinity of the Metal-Insulator Transition
Physical Review Letters 32, 769 (1974)
Supported by the National Science Foundation under Grant GH-33634

Peter M. Richards and M. B. Salamon
Exchange Narrowing of Electron Spin Resonance in a Two-Dimensional System
Physical Review B9, 32 (1974)
Supported by the National Science Foundation under Grant GH-33634 and the U. S. Atomic Energy Commission (Sandia)

M. B. Salamon
Evidence for Dipolar-Dominated Critical Behavior in EuO
Solid State Communications 13, 1741-1745 (1973)
Supported by the National Science Foundation under Grant GH-33750

F. L. Lederman, M. B. Salamon, and L. W. Shacklette
Experimental Verification of Scaling and test of the Universality Hypothesis from Specific-Heat Data
Physical Review B9, 2981-2988 (1974)
Supported by the National Science Foundation under Grant GH-33750

M. B. Salamon
Critical Acoustic Relaxation in EuO
Physical Review Letters 30, 968-971 (1973)
Supported by the National Science Foundation under Grant GH-33750

D. S. Simons and M. B. Salamon
Magnetic Field Dependence of the Specific Heat and Resistivity of Gd near T_c
Proceedings of the International Conference on Magnetism, Moscow, 1973 (submitted to)
Supported by the National Science Foundation under Grant GH-33634

M. B. Salamon, P. R. Garnier, B. Golding, and E. Buehler
Simultaneous Measurement of the Thermal Diffusivity and Specific Heat near Phase Transitions
Journal of Physics and Chemistry of Solids (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-33750

M. B. Salamon and F. L. Lederman
Universality and the Critical Specific Heat of β-brass
Physical Review (Comments and Addenda) (submitted to)
Supported by the National Science Foundation under Grants GH-33634 and GH-33750

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Spin-Lattice Relaxation and Dynamic Nuclear Orientation

Principal Investigator: Harvey J. Stapleton, Ph.D.
Professor of Physics

Supporting Agency: National Science Foundation

Senior Staff: Harvey J. Stapleton, Professor

Junior Staff: Patrick Devaney, Research Assistant
Gordon E. Fish, Research Assistant
Richard C. Herrick, Research Assistant
Raymond Marchand, Research Assistant

Objectives: Our experiments are aimed at an understanding of the various interactions which influence the spin-lattice relaxation rate of rare earth ions and to apply this information, when possible, to the construction of devices which can dynamically polarize nuclei in solids. In the last year the emphasis has been to better understand:

1) the influence of hyperfine interactions on the spin-lattice relaxation of a Kramers transition;

2) a newly observed, magnetic-field-dependent, two-phonon relaxation process;

3) the interference between resonant and non-resonant two-phonon relaxation mechanisms;

4) the temperature dependence of a non-resonant Raman relaxation rate when an electronic state lies just beyond the phonon cut-off energy;

5) and ligand hyperfine interactions through electron nuclear double resonance (ENDOR) experiments.

Approach: The experimental approach to these relaxation questions involved making electron spin resonance measurements using both pulse-saturation and cw linewidth techniques near 9 and 16 GHz at controlled temperatures between 1.5 and 30 K. From the pulse saturation studies, the relaxation rate $1/T_1$, can be measured directly until T_1 is shorter than 50 microseconds. Then at higher temperatures T_1 shortens to less than 10^{-8} sec and the line broadens due to spin-phonon interactions to a frequency width characterized by $1/T_2$. Studying T_1 and T_2 as a function of temperature, magnetic field direction, paramagnetic ion concentration, and hyperfine state, provides the necessary data.

ENDOR measurements consist of monitoring a partially saturated EPR transition while simultaneously applying an RF magnetic field to induce transitions between the nuclear spin states under study.

Progress: (01 07 73 - 30 06 74) Hyperfine Influence on $1/T_1$--We have corrected errors in two papers in the literature concerning these influences and have presented data on two salts of Er^{167} in which the dominant relaxation process involved allowed EPR transitions in one case, and forbidden EPR transitions in the other. Only our corrections to the theory can explain the vast differences in the relaxation behavior of these two Er^{167} salts.

New Relaxation Process Observed--We have observed and analyzed a previously undetected two-phonon relaxation rate which varied as $H^2T^7\sin^2\theta$. This type of relaxation had always been considered too weak to observe because of the stronger T^9 rate which must also be present. The process was observed in Nd-doped yttrium ethyl sulfate.

Interference Effects Among Two-Phonon Relaxation Mechanisms--A theoretical paper was completed which gives the temperature dependence of the interference terms between a T^9 non-resonant Raman relaxation mechanism and a resonant Raman (Orbach) process varying as $(\exp(\Delta/kT) - 1)^{-1}$.

Quasi-Resonant Raman Process--The Raman relaxation rate of U^{3+} in $LaCl_3$ was found to have a temperature dependence varying faster than T^9. A satisfactory explanation results if the phonon energies are not neglected in comparison to the excited electronic energies, since in this salt the first excited state lies slightly above the phonon cut-off energy.

ENDOR--A sensitive ENDOR spectrometer is under construction and works successfully on ionic crystals, but is not yet yielding data on frozen enzyme solutions.

Publications: (01 07 73 - 30 06 74)

R. L. Lichti and H. J. Stapleton
Proton Polarization and Relaxation in Ytterbium Doped Yttrium Hydroxide
Physical Review B8, 4134-4148 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

R. L. Marchand and H. J. Stapleton
Observation of an $H^2T^7\sin^2\theta$ Raman Spin-Lattice Relaxation Rate in a Neodymium Salt
Physical Review B9, 14-21 (1974)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

William T. Gray IV and H. J. Stapleton
Spin-Lattice Relaxation Rates for Nd^{3+}, Er^{3+}, and Ce^{3+} in $LaCl_3$ between 2.7 and 29 K
Physical Review B9, 2863-2869 (1974)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

R. L. Marchand
Contribution of Two Phonon Processes to the Spin-Lattice Relaxation Rate of Kramers Ions
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

H. J. Stapleton, R. L. Marchand, and E. R. Lemar
Hyperfine Effects on Spin-Lattice Relaxation Rates of Rare Earth Salts: Theory and Experimental Data
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

R. L. Marchand, G. E. Fish, and H. J. Stapleton
Spin-Lattice Relaxation of Trivalent Uranium in Anhydrous Lanthanum Trichloride
Physical Review (submitted to)
Supported by the National Science Foundation under Grant GH-33634

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Raymond Louis Marchand (H. J. Stapleton, Adviser)
Spin-Lattice Relaxation of Trivalent Cerium Neodymium and Erbium in Yttrium Ethyl Sulfate
February 1974
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

Diffraction Studies of Solids

Principal Investigator: Galen D. Stucky, Ph.D.
Professor of Inorganic Chemistry

Supporting Agency: National Science Foundation

Senior Staff: Galen D. Stucky, Professor
Arthur J. Schultz, Research Associate

Junior Staff: Jim Davis, NSF Fellow
Gerald Delker, Research Assistant
Benjamin Fieselmann, Teaching Assistant
Rudolph Jungst, Research Assistant
Robert I. Mink, Teaching Assistant
Dennis Sekutowski, NSF Fellow
Mamoru Tachikawa, UI Fellow
Michael Walczak, Research Assistant

Objectives: The objectives of this research program are to (1) synthesize and study the electronic properties of compounds which are structurally anisotropic in one or two dimensions and which exhibit unusual electron transfer properties; (2) isolate and characterize highly reactive organometallic intermediates which are essential to polymerization and catalytic processes: (3) experimentally investigate the rearrangement which occurs in valence electron distributions in the process atoms → molecules.

Approach: Low temperature neutron and X-ray diffraction techniques are used to independently determine the scattering effects due to the thermal motions of atoms and to aspherical electron distributions. The same techniques are being used to study dynamic structural processes in single crystals of organic and inorganic "metals". The electronic properties of these materials are being investigated in collaboration with Professors Myron Salamon, Miles Klein, and Charles Slichter of this Laboratory by a variety

of techniques. Organometallic species which are important as polymerization catalysts and as synthetic intermediates are synthesized, isolated and characterized by magnetic resonance and diffraction methods. The materials are subsequently evaluated for their chemical utility by investigating their reactions with a variety of substrates.

Progress: (01 07 73 - 30 06 74) (A) The three dimensional x-ray scattering from single crystals of silicon have been measured at liquid helium temperatures and the deviation of the valence electron density from spherical symmetry about the silicon atom determined (with R. Simmons and W. Hardy of the Department of Physics). Efforts are now being made to determine if it is feasible to directly measure charge distributions in first row transition metal molecular complexes.

(B) The compound tetrathiofulvalene tetracyanoquinodimethane has been synthesized and the dynamic structural properties investigated by single crystal and polycrystalline low temperature x-ray crystallography. No change in the periodicity of the lattice has been observed through the metal-semiconductor transition temperature, however some evidence for small structural changes in the vicinity of the transition temperature are observed. Further studies are in progress. A new one dimensional metallic complex, (guanidinium)$Pt(CN)_4Br_{0.3}$, has been synthesized. The conductivity of this material and its structure have been determined.

The above studies are directed towards the development of new one and two dimensional materials which have unusual electron transfer properties.

Publications: (01 07 73 - 30 06 74)

Ting-i Li, G. D. Stucky, and G. L. McPherson
The Crystal Structure of $CsMnCl_3$ and a Summary of the Structures of RMX_3 Compounds
Acta Crystallographica B29 (6), 1330-1335 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency

Yu Wang and G. D. Stucky
Bonding and Valence Electron Distributions in Molecules. The Crystal and Molecular Structure of 1,1,2,2-Tetracyanocyclopropane
Acta Crystallographica B29 (6), 1255-1258 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency

Ting-i Li and G. D. Stucky
The Effect of Exchange Coupling on the Spectra of Transition Metal Ions. The Crystal Structure and Optical Spectrum of $CsCrBr_3$
Acta Crystallographica B29 (6), 1529-1532 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency

Richard P. Zerger and G. D. Stucky
Synthesis and Crystal Structure of Bicyclo[1.1.0]Butyllithium Tetramethylethylenediamine
Journal of the Chemical Society (Chemical Communications)(Burlington House, London, 1973) pp. 44-45
Supported by the National Science Foundation under Grants GH-33634 and 31016X and the Advanced Research Projects Agency under Contract HC-15-67-C-0221

F. V. Hanson, R. C. Hazell, C. Hyatt, and G. D. Stucky
The Crystal and Molecular Structure of Tetramethylammonium 3,3'-Commo-bis [1,2-dicarbo-3-nickelaclosododecaborate][1-]
Acta Chemica Scandinavica 27, 1210-1218 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency

Gordon Sproul and G. D. Stucky
Stabilization of the Higher Oxidation States of Nickel: The Molecular Structure of Bis(2,6-diacetylpyridine-dioximato)Nickel(IV)
Inorganic Chemistry 12, 2898-2902 (1973)
Supported by the National Science Foundation under Grant GH-33634

G. L. McPherson, R. C. Koch, and G. D. Stucky
The Electron Spin Resonance Spectra of V^{2+}, Mn^{2+}, and Ni^{2+} in Single Crystals of $CsMgBr_3$ and $CsMgI_3$
Journal of Chemical Physics 60, 1424-1428 (1974)
Supported by the National Science Foundation under Grant GH-33634

R. A. Craven, M. B. Salamon, G. DePasquali, R. M. Herman, G. D. Stucky, and A. Schültz
The Specific Heat of Tetrathiafulvaliniumtetracyanoquinodimethane in the Vicinity of the Metal-Insulator Transition
Physical Review Letters 32, 1769 (1974)
Supported by the National Science Foundation under Grant GH-33634

Yu Wang, G. D. Stucky, and Jack M. Williams
Is Squaric Acid Square?: A Combined X-ray and Neutron Diffraction Study of 3,4-dihydroxy-3-cyclo-butene, 1,2-dione, $H_2C_4O_4$
Journal of the Chemical Society, Perkin Transactions II, 35-38 (1974)
Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Atomic Energy Commission (Argonne)

Galen Stucky
Stereochemical Properties of N-Chelated Alkali Metal Complexes
Advances in Chemistry Series 130, 56-112 (1974) (American Chemical Society Press, Washington, D.C.)
Supported by the National Science Foundation under Grants GH-33634 and GP-31016X

Galen D. Stucky, Arlene Mootz McPherson, W. E. Rhine, John J. Eisch, and John L. Considine
The Crystal Structure and Auto-Reactivity of the Diphenyl-(phenylethynyl)-aluminum Dimer: A Model for π-Complexation between Alkynes and Organoaluminum Compounds
Journal of The American Chemical Society 96, 1941-1942 (1974)
Supported by the National Science Foundation under Grants GH-33634 and GP-31016K (Illinois) and NSF GP-28209 (State University of New York)

Yu Wang and Galen Stucky
Some Comments on the Bonding in Three Membered Ring Systems and Transition Metal Olefin Complexes
Inorganic Chemistry (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Rudolph Jungst and Galen Stucky
A Mono-bridged Inner Sphere Dimer. The X-ray Crystal Structure of μ-cyanobis (5,7,7,12,14,14-hexamethyl 1,4,8,11-tetraazacyclotetradeca-4,11,-diene) dicopper(II)perchlorate
Inorganic Chemistry (submitted to)
Supported by the National Science Foundation under Grant GH-33634

H. Yasuda, M. Walczak, W. Rhine, and C. Stucky
The Oxidation Reactions of Organolithium-N,N,N',N'-tetramethylethylenediamine Complexes
Journal of Organometallic Chemistry (submitted to)
Supported by the National Science Foundation under Grant GH-33634

R. Zerger, W. Rhine, and G. D. Stucky
π Groups in Ion Pair Bonding. The Effect of the Cation on the Fluorenyl Ion Pairs
Journal of the American Chemical Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Yu Wang and G. D. Stucky
The Squaric Acid Molecule: A Hydrogen Bond Study of Dimethyl-ammonium-hydro-bis-bi-squarate, $[H_2N(CH_3)_2]\cdot H_3(C_4O_4)_2$
Journal of the Chemical Society, Perkin II (submitted to)
Supported by the National Science Foundation under Grant GH-33634

D. Michael Duggan, R. G. Jungst, K. R. Mann, G. D. Stucky, and D. N. Hendrickson
Electronic and Crystallographic Study of Two Cyanide-Bridged Copper(II) Dimers. Magnetic Exchange Interactions Through a Linear Cu-CN-Cu Bridge and a Hydrogen Bonded Cu-CN···H-N-Cu System
Journal of the American Chemical Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by HEW PHS HL13652

Richard Zerger, Wendell Rhine, and Galen Stucky
The Stereochemistry of Polynuclear Compounds of the Main Group Elements. The Bonding and Molecular Structure of Cyclohexyllithium, a Hexameric Organolithium Compound
Journal of the American Chemical Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634

Richard Zerger and Galen Stucky
Unsaturated Organometallic Compound of the Representative Elements. Biscyclopentadienyl Calcium
Journal of Organometallic Chemistry (submitted to)
Supported by the National Science Foundation under Grant GH-33634

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Richard Paul Zerger (G. Stucky, Adviser)
Bonding and Stereochemical Studies of Group IA and IIA Organometallic Compounds
October 1973
Supported by the National Science Foundation under Grants GH-33634 and GP-31016X and by the Advanced Research Projects Agency

Yu Wang (G. Stucky, Adviser)
Structural and Bonding Properties of Small Ring Compounds
October 1973
Supported by the National Science Foundation under Grant GH-33634

Physical and Catalytic Properties of Oxides

Principal Investigator: Gerald P. Wirtz, Ph.D.
Associate Professor of Ceramic Engineering
and Assistant Dean, College of Engineering

Supporting Agency: National Science Foundation

Senior Staff: Gerald P. Wirtz, Associate Professor

Junior Staff: John J. Janecek, Research Assistant
Vishwa N. Shukla, Research Assistant
Chyang J. Yu, Research Assistant

Objectives: To grow oxide single crystals for physical property measurements. To determine the thermodynamic properties of catalytic oxides. To investigate the mechanism of oxidation catalysis on oxides by isotopic exchange measurements. To correlate the physical and chemical properties of oxides with catalytic activity.

Approach: Liquid-solid phase equilibrium studies in rare earth-transition metal oxide systems. To investigate the feasibility of growing crystals from the liquid phase. Annealing of Tl_2O_3 crystals in oxygen permeable cells to vary defect concentration while controlling vaporization. Identification of gaseous reaction products by mass spectrography. Characterization of solid oxides by electrical conductivity and Hall effect, magnetic susceptibility, thermogravimetric analysis, and x-ray diffraction. Measurement of thermodynamic potentials by EMF measurements across a solid electrolyte.

Progress: (01 07 73 - 30 06 74) A high temperature thermal cell permitting visual examination during thermal analysis has been constructed for rapid liquid-solid phase studies at temperatures in excess of 1600°C. A

catalytic reactor coupled with a mass spectrograph has been constructed and is presently being used to analyze gases desorbed from ceramic powders at high temperatures. Chemical and physical changes in $LaCoO_3$ subjected to IC engine exhaust have been determined. The precipitation of Co metal from $LaCoO_3$ has been quantitatively determined by magnetic measurements and correlated with oxygen deficiency determined by thermogravimetric measurements. The catalytically active phase has been shown to be the perovskite phase containing both cation and anion vacancies. Similar measurements on Co_3O_4 and Sr doped $LaCoO_3$ and comparison of catalytic activities indicate that the active sites are oxygen vacancies. Efforts to obtain thermodynamic oxygen potentials by electrolytic cell measurements for correlation with catalytic activity are underway.

Publications: (01 07 73 - 30 06 74)

L. B. Sis, G. P. Wirtz, and S. C. Sorenson
Structure and Properties of Reduced $LaCoO_3$
Journal of Applied Physics 44, 5553-5559 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-G10

L. B. Sis, S. D. Brown, Tran Bho Van, and G. P. Wirtz
Polymorphic Phases in Anodic Spark Deposited Coatings of Al_2O_3
Journal of the American Ceramic Society 57, 108 (1974)
Supported by the American Gas Association

S. C. Sorenson, J. A. Wronkiewicz, L. B. Sis, and G. P. Wirtz
Properties of $LaCoO_3$ as a Catalyst in Engine Exhaust Gases
Bulletin of the American Ceramic Society (submitted to)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract SD-131

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Jerzy B. Niklewski (J. A. Nelson, Adviser)
Measurement of Adsorbate Evolution Temperatures and of Adsorbate Effects on Processing and Fired Properties of Submicron Alumina
June 1974
Supported by the National Science Foundation under Grant GH-33634

Jonathan S. Wheeler (G. P. Wirtz, Adviser)
Tungsten Trioxide-Molybdenum Trioxide Oxidation Catalysis
October 1973
Supported by Quaker Oats

ADVANCED RESEARCH PROJECTS AGENCY

Light Scattering in Solutions of Polymers, Macromolecules, Dense Gases, Liquids, and Liquid Crystals

Principal Investigator: Willis H. Flygare, Ph.D.
Professor of Chemistry

Supporting Agency: Advanced Research Projects Agency

Senior Staff: Willis H. Flygare, Professor
Gregory P. Alms, Research Associate
Ilan Chabay, Postdoc Biophysical Trainee
Steven Durana, Research Associate, NSF

Junior Staff: Sidney Bertucci, Research Assistant
Alan Burnham, Teaching Assistant
Timothy D. Gierke, Research Assistant
Steve Hartford, NSF Trainee
Yoshiaka Ishizu, Japanese National (Term 5/20/74)
Tilak Raj, Biophysical Trainee

Objectives: The general objectives are to study the interactions of molecules in dense gases, liquids, liquid crystals, and solutions. We are interested in the forces of interaction and dynamics between molecules and atoms in liquids and solids. In addition, we are interested in the hydrodynamic properties of macromolecules and polymers in solution.

Approach: The primary approach in our study is to analyze the frequency spectrum and intensities of light scattering from the various systems described above. The spectrum of the light contains information about the dynamics of motion in the scattering systems. The intensities obtained from the integrated spectrum gives information about the static correlations in the system. We are studying both positional and orientational static and dynamic correlations.

Progress: (01 07 73 - 30 06 74) We have made significant progress during this last year in studying the orientational pair correlations in several liquid crystal-like systems. By studying the spectrum of the depolarized light in the isotropic liquid phase of liquid crystal-like molecules (and the dilution dependence in carbon tetrachloride) we can relate the onset of liquid crystal phase to a critical density. This work is being continued in a wide range of liquid crystal-like molecules in order to understand the nature of the attractive forces in liquid crystal systems. We have also made progress in understanding the nature and the effects of the nonspherical Lorentz correction to the intensity of the scattered light in binary systems.

Publications: (01 07 73 - 30 06 74)

W. H. Flygare and T. D. Gierke
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Annual Review of Materials Science 4 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

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Applied Optics 12, 2838-2844 (1973)
Supported by the National Science Foundation under Grant GH-33634

J. C. McGurk, T. G. Schmalz, and W. H. Flygare
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Advanced Chemical Physics XX, Edited by I. Prigogine and S. A. Rice, (John Wiley and Sons, 1974)
Supported by the National Science Foundation under Grants GH-33634 and GP-12382X3

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Journal of Physical Chemistry of Solids 34, 1199-1208 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC15-71-0253, University of Michigan

H. Jetter, E. F. Pearson, C. L. Norris, J. C. McGurk, and W. H. Flygare
Time Resolved Infrared-Microwave Double Resonance in $^{13}CH_3F$; Theory and Experiment
Journal of Chemical Physics 59, 1796-1805 (1973)
Supported by the National Science Foundation (Non-MRL)

J. C. McGurk and W. H. Flygare
The Detection and Assignment of the Microwave Spectrum of IF
Journal of Chemical Physics 59, 5742-5744 (1973)
Supported by the National Science Foundation (Non-MRL)

C. L. Norris, E. F. Pearson, and W. H. Flygare
The Molecular Zeeman Effect in Methyl Fluoride
Journal of Chemical Physics 60, 1758-1761 (1974)
Supported by the National Science Foundation (Non-MRL)

E. F. Pearson, C. L. Norris, and W. H. Flygare
Molecular Zeeman Effect, Electric Dipole Moment, and Boron Nuclear Hyperfine Coupling Constants in HBS
Journal of Chemical Physics 60, 1761-1770 (1974)
Supported by the National Science Foundation (Non-MRL)

S. L. Rock, E. F. Pearson, E. Appleman, C. L. Norris, and W. H. Flygare
The Molecular Rotational Zeeman Effect in HOF, a Comparison with H_2O F_2O_1 and other Fluorine Containing Molecules; and Dipole Moments of HOF and DOF
Journal of Chemical Physics 59, 3940-3947 (1973)
Supported by the National Science Foundation (Non-MRL)

T. G. Schmalz, C. L. Norris, and W. H. Flygare
Localized Magnetic Susceptibility Anisotropies
Journal of the American Chemical Society 95, 7961-7974 (1973)
Supported by the National Science Foundation (Non-MRL)

W. H. Flygare
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Advances in Chemistry, Critical Evaluation of Chemical and Physical Structural Information, Edited by D. R. Lide and C. K. Johnson, 1974
Supported by the National Science Foundation (Non-MRL)

J. L. McGurk, C. L. Norris, T. G. Schmalz, E. F. Pearson, and W. H. Flygare
Infrared-Microwave Double Resonance Measurements of T_1 in Methyl Fluoride and Methyl Chloride
Proceedings of the First International Symposium of Laser Spectroscopy, 1973, Edited by A. Moradian and R. Brewer
Supported by the National Science Foundation (Non-MRL)

T. D. Gierke and W. H. Flygare
Depolarized Raleigh Scattering in Liquids: Molecular Reorientation and Orientation Pair Correlations in a Nematic Liquid Crystal: MBBA
Journal of Chemical Physics (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

J. C. McGurk, T. G. Schmalz, and W. H. Flygare
Fast Passage in Rotational Spectroscopy: Theory and Experiment
Journal of Chemical Physics (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

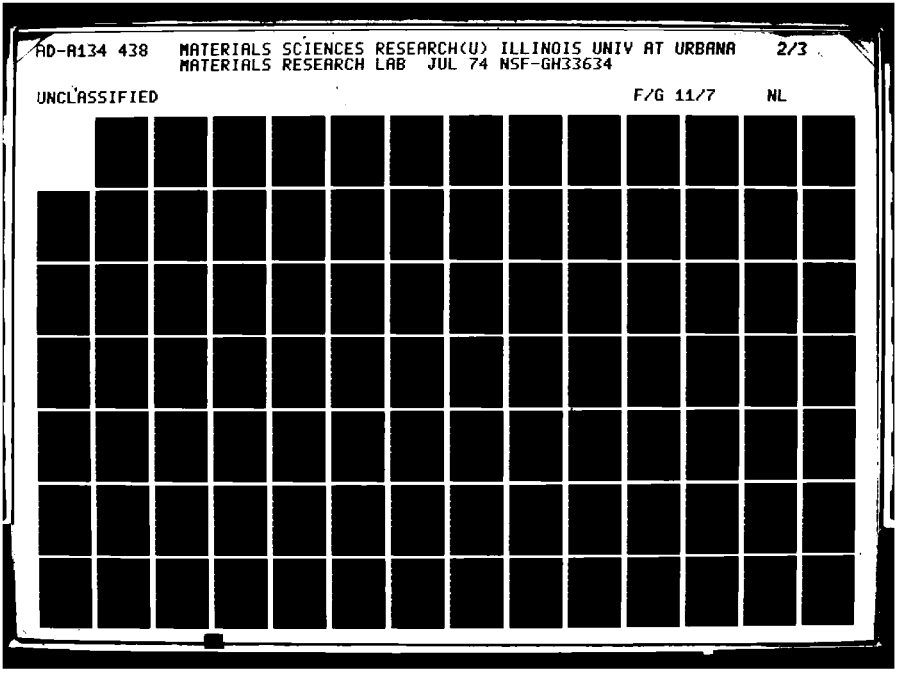
W. H. Flygare and B. R. Ware
Analysis of Polymer Mixtures in Solution Utilizing Electrophoretic Light Scattering Apparatus
United States Patent No. 3,766,048, October 16, 1973

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

C. L. Norris (W. H. Flygare, Adviser)
Molecular Zeeman Effect Studies and Time Resolved Infrared-Microwave Double Resonance
August 1973
Non-MRL Supported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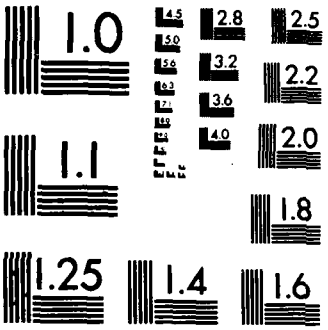

Luminescence, Lasers, Carrier and Impurity Effects in Compound Semiconductors

Principal Investigator: Nick Holonyak, Jr., Ph.D.
Professor of Electrical Engineering

Supporting Agency: Advanced Research Projects Agency

Senior Staff: Nick Holonyak, Jr., Professor
Joe C. Campbell, IBM Postdoctoral Fellow

Junior Staff: W. R. Hitchens, Research Assistant
Michael H. Lee, Research Assistant
M. J. Ludowise, Research Assistant
J. J. Coleman, Research Assistant, NSF
R. J. Nelson, Research Assistant, NSF

Objectives: Study III-V compounds, isoelectronic traps and complexes, spontaneous and stimulated recombination, luminescence, lasers, p-n junctions, and heterojunctions.

Approach: Crystal growth and junction formation by vapor transport, growth from solution (constant-temperature liquid-phase epitaxy [CT-LPE]), and impurity diffusion. Electrical and optical measurements (4.2-300°K) on thin homogeneous samples and on p-n junctions.

Progress: (01 07 73 - 30 06 74) Extensive work on nitrogen-doped $GaAs_{1-x}P_x$ and on CT-LPE $In_{1-x}Ga_xP$ has been carried out. With Verdeyen's group (EE) we have shown that $x = 0.47$ $GaAs_{1-x}P_x$:N can be pumped with an electron beam generated by a gas plasma and can be operated as a laser on the A-line recombination transition. If the N-doped layer is removed from the sample, the crystal proves to be indirect in its behavior. The effect of the Zn acceptor in direct and indirect $GaAs_{1-x}P_x$:N has been determined experimentally and theoretically. Beyond the direct-indirect transition, holes bound to

the Zn acceptor are not involved in recombination with electrons bound to the N (or NN) isoelectronic trap because of insufficient overlap of the electron and hole wave functions. The effect of decreasing of $GaAs_{1-x}P_x$:N crystal composition below x = 1 and thus the increase of the k = 0 wave function component of the electron bound to the N trap has been determined and shows that an optimum LED can be approached in the crystal composition range 0.6-0.8. That is, for a comparable state of the crystal and junction art for GaP:N and $GaAs_{1-x}P_x$:N, GaP does not prove to be the right choice for a general purpose LED. The ternary exceeds the performance of the binary, as has been verified theoretically in this project and experimentally by Craford and co-workers (Monsanto). In addition to the above work, we have measured in $GaAs_{1-x}P_x$:N and $In_{1-x}Ga_xP$ the carrier lifetime in both the spontaneous and stimulated regimes as a function of recombination-radiation wavelength. A major change (decrease) in carrier lifetime is resolved in the region of stimulated emission.

Publications: (01 07 73 - 30 06 74)

R. D. Dupuis, N. Holonyak, Jr., M. H. Lee, J. C. Campbell, M. G. Craford, D. Finn, and D. L. Keune
Laser Operation of $GaAs_{1-x}P_x$:N (x=0.37, 77°K) on Photopumped NN_3 Pair Transition
Applied Physics Letters 22, 369-371 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, and by the National Science Foundation under Grant GH-33771

J. T. Verdeyen, W. L. Johnson, B. E. Cherrington, N. Holonyak, Jr., J. C. Campbell, M. H. Lee, and M. G. Craford
Electron-Beam Pumped Semiconductor Laser Using a Gas Plasma Gun (GPG)
Applied Physics Letters 23, 102-103 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grants GH-33771 and GK-27559, and by the U. S. Army Night Vision Lab

H. M. Macksey, M. H. Lee, N. Holonyak, Jr., W. R. Hitchens, R. D. Dupuis, and J. C. Campbell
Crystal and Luminescence Properties of Constant-Temperature Liquid-Phase-Epitaxial $In_{1-x}Ga_xP$ (x~0.7) Grown on (100) $GaAs_{1-x}P_x$ (x~0.4)
Journal of Applied Physics 44, 5035-5040 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GH-33771, and by the U. S. Army Night Vision Lab

C. B. Duke and N. Holonyak, Jr.
Advances in Light Emitting Diodes. Traps and Resonance in III-V Ternary Alloys: A New Dimension in Semiconductor Light
Physics Today 26, 23 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

J. C. Campbell, N. Holonyak, Jr., M. H. Lee, M. J. Ludowise, M. G. Craford, D. Finn, and W. O. Groves
Recombination Transitions in Zn-N-Doped $GaAs_{1-x}P_x$ in the Direct and Indirect Composition Regions
Journal of Applied Physics 45, 795-799 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, and by the National Science Foundation under Grant GH-33771

N. Holonyak, Jr., J. C. Campbell, M. H. Lee, J. T. Verdeyen, W. L. Johnson, M. G. Craford, and D. Finn
Pumping of $GaAs_{1-x}P_x$:N (at 77°K, for $x \leq 0.53$) by an Electron Beam from a Gas Plasma
Journal of Applied Physics 44, 5517-5521 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grants GH-33771, GK-37759, and by the U. S. Army Night Vision Lab under Contract DAAK-02-72-C-0076

M. H. Lee, N. Holonyak, Jr., J. C. Campbell, W. O. Groves, M. G. Craford, and D. L. Keune
Spontaneous and Stimulated Carrier Lifetimes (77°K) in $GaAs_{1-x}P_x$:N
Applied Physics Letters 24, 310-313 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, and the National Science Foundation under Grant GH-33771

J. C. Campbell, W. R. Hitchens, N. Holonyak, Jr., M. H. Lee, M. J. Ludowise, and J. J. Coleman
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Applied Physics Letters 24, 327-330 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

M. H. Lee, N. Holonyak, Jr., J. C. Campbell, W. O. Groves, and M. G. Craford
Behavior of Above-Gap NN-Pair States in Radiative Recombination in $GaAs_{1-x}P_x:N^+$ ($x=0.24$, 77°K)
Journal of Applied Physics 45, 1775-1778 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10 and by the National Science Foundation under Grant GH-33771

J. C. Campbell, N. Holonyak, Jr., A. B. Kunz, and M. G. Craford
Model Calculations for Radiative Recombination in Zn-N-Doped $GaAs_{1-x}P_x$ in the Direct and Indirect Composition Region
Physical Review B (May 15) (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grants GH-33634 and GH-33771, and by the Aerospace Research Lab, USAF AFB Contract F-33615-72-C-1506

W. R. Hitchens, N. Holonyak, Jr., M. H. Lee, and J. C. Campbell
Liquid Phase Epitaxial Growth and Photoluminescence Characterization of Laser-Quality (100) $In_{1-x}Ga_xP$
Journal of Crystal Growth (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

J. C. Campbell, N. Holonyak, Jr., A. B. Kunz, and M. G. Craford
Effect of Crystal Composition on "Quasi-Direct" Recombination and LED Performance in Indirect Region of $GaAs_{1-x}P_x:N$
Applied Physics Letters 25, (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grants GH-33634 and GH-33771, and the Aerospace Research Laboratory

M. H. Lee, N. Holonyak, Jr. W. R. Hitchens, J. C. Campbell, and M. Altarelli
The Direct-Indirect Transition $In_{1-x}Ga_xP$
Solid State Communications (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GH-33771, by the U. S. Army Night Vision Lab DAAK-02-72-C-0076, and by the U. S. Army Research Office under Contract DAHC-04-74-C-0005

J. C. Campbell, N. Holonyak, Jr., M. G. Craford, and D. L. Keune
Band Structure Enhancement and Optimization of Radiative Recombination in $GaAs_{1-x}P_x:N$ (and $In_{1-x}Ga_xP:N$)
Journal of Applied Physics (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, and by the National Science Foundation under Grant GH-33771

W. R. Hitchens, N. Holonyak, Jr., M. H. Lee, J. C. Campbell, J. J. Coleman, W. O. Groves, and D. L. Keune
Liquid Phase Epitaxial (LPE) Grown-Junction $In_{1-x}Ga_xP$(x~0.63) Laser of Wavelength λ~5900 Å (2.10 eV, 77°K)
Applied Physics Letters (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GH-33771, and by the U. S. Army Night Vision Lab DAAK-02-72-C-0076

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Joe Charles Campbell (N. Holonyak, Jr., Adviser)
Indium Gallium Arsenide and Indium Phosphide Injection Lasers and Radiative Recombination in Nitrogen-Zinc-Doped Gallium Arsenide Phosphide
October 1973
Supported by the Advanced Research Projects Agency under Contract HC-15-67-C-0221, by the National Science Foundation under Grants GK-18960 and GH-33771, by the University Industrial Affiliates Program, Night Vision Lab DAAK-02-73-C-0076, and by JSEP DAAB-07-67-C0199

High-Pressure Nuclear Magnetic Resonance and Raman Study of the Dynamic Structure of Liquids, Disordered Solids and Polymers

Principal Investigator: Jiri Jonas, Ph.D.
Professor of Chemistry

Supporting Agency: Advanced Research Projects Agency

Senior Staff: Jiri Jonas, Professor

Junior Staff: John H. Campbell, Research Assistant
Yun-Ko Lee, Research Assistant (Term 10/10/73)
Hugh J. Parkhurst, Research Assistant
David J. Wilbur, Research Assistant

Objectives: The general aim of the research is to improve our understanding of the dynamic structure of liquids, disordered solids and polymers by investigation of motions and interactions at the molecular level. In a systematic way we attempt to obtain experimental data which will enable us to draw conclusions of general validity about the reorientation mechanism and transport properties of liquids. In the area of disordered solids the main interest is in the nature of the order-disorder transitions and the hysteresis effects accompanying such transitions. Preliminary studies of elastomers are directed towards elucidation of the relationship between the dynamic structure and the mechanical properties of polymers.

Approach: The most important feature in all our experiments is that we use both pressure and temperature as experimental variables which enables us to separate the effects of density and temperature on the dynamic processes studied. In particular the constant density experiments are important as

a means to obtain information about the true effect of temperature on the dynamic process. Several experimental techniques are used to investigate the molecular motions and interactions in the materials of interest: (1) Nuclear magnetic resonance spin-lattice relaxation times are measured over a wide range of temperatures and pressures. (2) The NMR spin echo method using the fixed magnetic field gradient is employed to determine diffusion coefficients. (3) Fourier transform deconvolution technique is used to obtain the time dependence of reorientational and vibrational correlation functions from laser Raman band shapes. (4) Shear viscosities and PVT data are also studied in liquids.

Progress: (01 07 73 - 30 06 74) (1) Both Raman and NMR techniques were used in a detailed investigation of the molecular motions of a symmetric-top molecule methyl iodide-d_3 in the liquid state. The method of Fourier transform deconvolution was used to obtain the correlation functions from the Raman spectra. For the first time it was possible to separate the effects of density and temperature on the reorientational correlation functions and the vibrational correlation functions. All results show the dominant effect of density on molecular motions. On the basis of this study, we concluded that the model of a hard sphere liquid, the assumption of binary collisions and the temperature dependence of the hard sphere diameter appear to be promising concepts leading to a better description of the liquid state.

(2) NMR studies of spin rotation interaction relaxation mechanism provide unique information about the angular momentum in liquids. One determines

the angular momentum correlation time, τ_J, which corresponds to the time it takes the molecule to lose memory of its initial angular momentum. There are two important results of our studies. First, the Gordon J-diffusion model describes well the reorientation of molecules not only in dense fluids but also at supercritical temperatures and becomes equivalent to a perturbed free rotor model in the dilute gas limit. Secondly, for the first time, we were able to follow the temperature behavior of τ_J at constant density and found that experimental τ_J increases with increasing temperature at constant density. This finding is of particular interest because τ_J is related to the time between collisions. We interpreted the experimental data in terms of the Enskog theory and the cell model which were used to calculate the theoretical time between collisions (τ_{BC}). In order to obtain the correct prediction of the observed temperature change in τ_J ($\propto \tau_{BC}$) at constant density we had to assume a temperature dependence of the hard sphere diameter.

(3) As a part of our systematic effort to elucidate some of the problems of the dynamic structure of electrolyte solutions, we have finished a study of the effects of pressure and temperature on the dynamic structure of several electrolyte solutions. Both structure breaking and structure forming ions were investigated. The determination of motional behavior of water molecules in solvation shells of the ions was possible.

(4) The first results of our experiments on NMR relaxation in disordered solids show convincingly that these studies will be fruitful in investigating order-disorder transitions and the hysteresis effects accompanying such

transitions. By following the effect of temperature and pressure on relaxation in several polymers, e.g., we determined the pressure dependence of the glass transition temperature which information is of theoretical and practical interest.

(5) New experimental NMR setup, which enables us to measure the spin lattice relaxation times and diffusion coefficients at pressures up to 10 kbar and temperatures up to 300°C was built and tested. Measurements of heavy water and various electrolytic solutions are in progress.

Publications: (01 07 73 - 30 06 74)

J. Hyde Campbell, J. F. Fisher, and J. Jonas
Density and Temperature Effects on the Molecular Reorientation and Vibrational Relaxation in Liquid Methyl Iodide
Journal of Chemical Physics 60, (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

J. H. Campbell, S. J. Seymour, and J. Jonas
Reorientational and Angular Momentum Correlation Times in Gaseous Tetrafluoromethane at Moderate Densities
Journal of Chemical Physics 59, 4151-4156 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP28268X

J. Jonas
NMR Relaxation in Liquids and Liquid Crystals
Magnetic Resonance Review 2, 203-220 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-28268X

J. Jonas
NMR Studies in Liquids at High Pressure
Advances Magnetic Resonance 6, 73-139 (1973)
Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

Yun-Ko Lee, J. H. Campbell, and J. Jonas
Effect of Pressure on Deuteron Spin-Lattice Relaxation in Several Concentrated Deuterium Oxide Diamagnetic Electrolyte Solutions
Journal of Chemical Physics 60, 3537-3543 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

Y. Lee and J. Jonas
Pressure and Concentration Effects on the Molecular Reorientation in Water-Dioxane Mixtures
Journal of Chemical Physics 59, 4845-4854 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-28268X

J. DeZwaan, R. J. Finney, and J. Jonas
Molecular Motions of Fluorobenzene-d_5 in the Dense Fluid Region
Journal of Chemical Physics 60, 3223-3245 (1974)
Supported by the USAFOSR under Contract AF-72-2286

J. DeZwaan and J. Jonas
Effect of Pressure on the Overall and Internal Rotation in Liquid Benzyl Cyanide
Journal of Physical Chemistry 77, 1768-1772 (1973)
Supported by the National Science Foundation under Grant GP-28268X and by the USAFOSR under Contract AF-72-2286

J. Jonas, J. DeZwaan, and J. H. Campbell
Nuclear Magnetic Resonance Relaxation Studies of Reorientational Motions in Liquids at High Pressure
Proceedings of Conference (J. Lascombe, Ed., D. Riedel Publishing Co., Dordrecht, Holland, 1974) pp. 343-353
Supported by the National Science Foundation under Grant GP-28268X and by the USAFOSR under Contract AF-72-2286

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Yun Ko Lee (J. Jonas, Adviser)
High Pressure Nuclear Magnetic Resonance Studies of Hydrogen - Bonded Systems
January 1974
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10.

Light Scattering from Disordered Materials

Principal Investigator: Miles V. Klein, Ph.D.
Professor of Physics

Supporting Agency: Advanced Research Projects Agency

Senior Staff: Miles V. Klein, Professor
Wayne Wozniak, Research Associate
Valters Ziraps, Soviet Exchange Scholar (9/15/73-5/??/74)

Junior Staff: James E. Clemans, Research Assistant
Robert A. Field, Research Assistant and University Fellow
David Gallagher, Research Assistant
John A. Holy, Research Assistant

Objectives: To study light-scattering from hydrogen diffusing and vibrating in metals such as niobium (with H. K. Birnbaum). To perform similar measurements on inorganic salts containing rapidly diffusing ions. To study light scattering in glasses with emphasis on temperature-dependence of the Brillouin linewidth and on residual depolarized Rayleigh scattering. To study the infrared and Raman vibrations in organic charge-transfer complexes, especially those that show high conductivity.

Approach: Use of a double grating Raman spectrometer and single and triple-passed Fabry-Perot interferometer for the measurements of scattered-light spectra. Development of a special high-vacuum, controlled temperature, controlled atmosphere chamber for the metal samples. Obtain suitable crystals and sample mounts for temperature-dependent Raman studies above room temperature.

Progress: (01 07 73 - 30 06 74) The special chamber and samples are ready for the hydrogen-in-metals experiments. Some samples of highly conducting

salts are being prepared. Both systems require special techniques to reject stray light. These are being developed.

The glass experiments require an extremely stable Fabry-Perot interferometer. This system with its related equipment is being assembled.

We have recently obtained low temperature Raman spectra for single crystals of the highly conducting charge transfer complex TTF-TCNQ. Although we can report no dramatic differences between the spectra at room temperature and liquid He temperature, other facets of the spectra indicate significant changes in the TCNQ species in forming the complex.

In addition, we have begun a normal coordinate analysis on TTF, the other organic member of the complex. Infrared and Raman spectra of KBr pellets of TTF have been obtained and we are in the process of using this data to study the normal vibrations of this molecule. The results of these calculations will be used in conjunction with the previous vibrational analyses of TCNQ in the interpretation of the spectra of TTF-TCNQ.

A program of study of second-order Raman scattering and of impurity induced Raman scattering from solidified gases was begun in collaboration with Professor R. K. Crawford. The gases are solidified at high pressures to allow study of the density dependence of the scattering and to facilitate handling of these normally fragile specimens. Preliminary data have been obtained for the temperature and density dependences of the second order scattering from pure solid argon and for the impurity induced scattering from argon doped with krypton. Various other combinations of host material and impurities are contemplated.

Point defects produced by x-irradiation of KBr crystals at 5.2 K and recombination phenomena have been studied by simultaneous measurement of thermally stimulated currents (TSC) and depolarization currents (TCDS), optical absorption charges and non-isothermal bleaching curves. One goal was to determine the electrical charge state of the primary Frenkel defects produced by the x-irradiation, i.e. does the annihilation of radiation-produced electron-hole pairs or excitons cause charged (α-I) or neutral (F-H) primary disorder? Present results confirm earlier high temperature results that favor the charged-primary-defect processes.

Publications: (01 07 73 - 30 06 74)

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Nuclear Spin Relaxation and Knight Shift in Transition Metals
Physical Review B8, 1055-1060 (1973)
Supported by the National Science Foundation under Grant GH-33634

B. N. Ganguly
High Frequency Local Modes, Superconductivity and Anomalous Isotope Effect in PdH(D) Systems
Zeitschrift für Physik 265, 433-439 (1973)
Supported by the National Science Foundation under Grant GH-33634

B. N. Ganguly
The Gruneisen Constant for Hydrogen Mode in PdH System
Physics Letters 46A, 23-24 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10 and by the National Science Foundation under Grant GH-33634

Miles V. Klein
The Equivalence of Resonance Raman Scattering in Solids with Absorption Followed by Luminescence
Physical Review-Comments and Addenda 8, 919-921 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GP-28319

Judith G. Peascoe and Miles V. Klein
Raman Scattering by the Hydroxyl Ion in Sodium Chloride
Journal of Chemical Physics 59, 2394-2408 (1973)
Supported by the Advanced Research Projects Agency under Contract
DAHC-15-73-G10 and by the National Science Foundation under Grants
GP-11173 and GP-28319

Judith G. Peascoe, W. R. Fenner, and Miles V. Klein
Raman Scattering by the Hydroxyl Ion in KCl and KBr
Journal of Chemical Physics (submitted to)
Supported by the Advanced Research Projects Agency under Contracts
DAHC-15-73-G10 and HC-15-67-C-0221 and by the National Science Foundation
under Grants GH-33634, GH-37757, GP-11173, and GP-28319

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Liquid Crystals and Phase Transitions

Principal Investigator: William McMillan, Ph.D.
Professor of Physics

Supporting Agency: Advanced Research Projects Agency

Senior Staff: William McMillan, Professor

Junior Staff: Ravindra Bhatt, Research Assistant and University Fellow
Kung Chao Chu, Research Assistant
Chung-Shih Hsu, Research Assistant
Robert J. Meyer, Research Assistant
Mark P. Sears, Research Assistant

Objectives: We want to produce physical theories of the various liquid crystal phases and to subject the theories to rigorous experimental tests. The objective, broadly speaking, is to advance liquid crystal physics from its present rather primitive state to the advanced level of solid state physics.

Approach: Three theoretical approaches are being persued vigorously: (1) Microscopic theory based on a model intermolecular interaction treated within the mean field approximation; (2) Phenomenological (Landau) theories based on the order parameter dependence of the free energy. Both static and dynamic theories are possible; (3) Wilson theory of the critical behavior near a second order phase transition. The experimental approach being pursued at present is light scattering using the self-beating technique. Light scattering provides an experimental probe of the static and dynamic behavior of the liquid crystal director. Several theories of the second order smectic A-nematic phase transition are now available to be tested.

Progress: (01 07 73 - 30 06 74) (1) A microscopic theory of the smectic C, B, and H phases is completed. The theoretical results include a phase diagram for the smectic phases as well as predictions of the temperature dependence

of thermodynamic properties and order parameters.

(2) We are currently trying to construct a microscopic model of the two new phases of TBBA.

(3) A dynamic Landau theory of the smectic A-nematic phase transition has been constructed to explain the pretransition increase in the nematic viscosity coefficients recently observed.

(4) We are struggling with the problem of producing a dynamical theory in the critical region analogous to the static Wilson theory.

(5) The light scattering apparatus and an elaborate hot stage (with temperature control within $\pm$ 1 mK) have been constructed and tested. We are now learning to purify and control the liquid crystals so that measurements of elastic constants and viscosities can be made within a few millikelvin of the phase transition. This experiment will provide a rigorous test of the static and dynamic behavior of nematics near the transition to the smectic A phase.

The following two problems are only loosely related to the liquid crystal effort.

(6) We have found a new way Wilson theory. This is quantification of Kadanoff's block spin concept and we have developed the ideas by applying them to a calculation of the critical behavior of the two-dimensional Ising model.

(7) A theory of anomalous dispersion in liquid He^4 has been developed to explain propagation of high frequency phonons recently observed by Dynes and Naharanamurti.

Publications: (01 07 73 - 30 06 74)

W. L. McMillan
A Simple Molecular Theory of the Smectic C Phase
Physical Review A8, 1921-1929 (1973)
Supported by the National Science Foundation under Grant GH-33634

W. L. McMillan
Time Dependent Landau Theory for the Smectic A-Nematic Phase Transition
Physical Review A9, 1720-1724 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

W. L. McMillan
Molecular Order and Molecular Theories of Liquid Crystals
American Chemical Society Symposium on Ordered Fluids and Liquid Crystals
Chicago, 1973 (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Properties of Recombination Centers in Semiconductors

Principal Investigator: Chih-Tang Sah, Ph.D.
Professor of Electrical Engineering and of Physics

Supporting Agency: Advanced Research Projects Agency

Senior Staff: Chih-Tang Sah, Professor
Soong H. Lee, Visiting Research Assistant Professor
Chi-Tong Wang, Visiting Research Assistant Professor
Arnast Neugroschel, Visiting Research Associate

Junior Staff: Chak Lun Chie, Research Assistant
F. Hennig, Research Assistant
Thomas Y. Lo, Research Assistant
Chyan-Chang Shiue, Research Assistant
Phillip D. Wright, Research Assistant

Objectives: (1) To obtain highly accurate energy level schemes and macroscopic capture and emission rates of electrons and holes at imperfection centers in semiconductors. (2) To develop quantum mechanical theories to interpret these fundamental parameters from atomic models. (3) To use these results to predict the electrical and optical properties of silicon diodes, transitors, integrated circuits and compound semiconductor devices.

Approach: The macroscopic transition rates and energy level schemes of bound electrons and holes are measured from current and high frequency capacitance transients in p-n junctions after switching electrically, optically, or thermally. Theoretical quantum models and analyses are developed from a two parameter impurity potential, including the central cell effect, and from first principle impurity pseudopotentials derived from published self-consistent atomic potentials.

Progress: (01 07 73 - 30 06 74) The highly sensitive (better than 10^{11} centers per cm^3) depletion layer capacitance transient technique has been used to determine the origin of the double donor quench-in centers in silicon after high temperature processing. Results of extensive sets of experiments are designed in which the concentration of phosphorus and boron in the diffused layer, the diffusion temperature and times are varied. These experiments show that the centers are definitely associated with the presence of very high concentrations of surface layers of boron and phosphorus. It is also shown that these centers have very high diffusion coefficients and a formation energy of 2.2 eV. These results are consistent with the vacancy model proposed by us previously. Properties of Cr centers in silicon are also investigated using the capacitance transient on Schottky barriers made on chromium doped silicon. The junction capacitance method has also been used to determine the low-electric-field and thermal equilibrium values of the thermal capture and emission rates of electrons and holes at the gold donor and acceptor centers in silicon. Very high resistivity silicon is employed (1 to 10 K ohm-cm). New and reliable temperature and electric-field dependences of these rates are obtained and the temperature dependence of the thermal activation energy or energy level of these centers from the band edges are obtained. The mass action law has been verified to within a factor of two. Interfacing equipment has been built and assembled to provide online analysis of experimental data and successful operation has been achieved.

Publications: (01 07 73 - 30 06 74)

D. H. Eaton and C. T. Sah
Series Equivalent Circuit Representation of SiO_2-Si Interface and Oxide Trap States
Solid State Electronics 16, 841-846 (1973)
Supported by the National Science Foundation under Grants GH-33634 and GK-30283, by the Advanced Research Projects Agency under Contract HC-15-67-0221, and by AFOSR-71-2067

J. M. Herman III and C. T. Sah
Thermal Capture of Electrons and Holes at Zinc Centers in Silicon
Solid State Electronics 16, 1133-1139 (1973)
Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract HC-15-67-C-0221, and by AFOSR-71-2067

K. Hess and C. T. Sah
Hot Carriers in Silicon Surface Inversion Layers
Journal of Applied Physics 45, 1254-1257 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10 and by AFOSR-71-2067

M. J. McNutt and C. T. Sah
High Frequency Space Charge Layer Capacitance of Strongly Inverted Semiconductor Surfaces
Solid State Electronics 17, 377-385 (1974)
Supported by the National Science Foundation under Grants GH-33634 and GK-30283, and by AFOSR-71-2067

T. H. Ning and C. T. Sah
Effects of Inhomogeneities of Surface-Oxide Charges on the Electron Energy Levels in a Semiconductor Surface-Inversion Layer
Physical Review B9, 527-535 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GH-33634, and by AFOSR-71-2067

C. T. Sah and H. S. Fu
Transient Response of MOS Capacitors Under Localized Photoexcitation
IEEE Trans ED-21, 202-209 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grants GH-33634 and GK-30283, and by AFOSR-71-2067

C. T. Sah and F. A. Lindholm
Transport in Semiconductors with Low Scattering Rate and at High Frequencies
Solid State Electronics 16, 1447 (1973)
Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract HC-15-67-C-0221, and by AFOSR-71-2067

C. T. Smiley, L. D. Yau, and C. T. Sah
Application of the Transmission Line Equivalent Circuit Model to the Analysis of the pn Junction Admittance Under dc Bias
Solid State Electronics 16, 895-901 (1973)
Supported by the Advanced Research Projects Agency under Contract HC-15-67-C-0221, by the National Science Foundation under Grant GK-30283, and by AFOSR-71-2067

J. W. Walker and C. T. Sah
Spherical-Square-Well Defect-Potential Model for 1-MeV Electron Irradiated Defects in Silicon
Physical Review B8, 5597-5603 (1973)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GH-33634, and by AFOSR-71-2067

J. W. Walker and C. T. Sah
Characteristics of 1.0 MeV Electron-Irradiated Surface-Controlled Silicon Junction Diodes
Radiation Effects 20, 187-195 (1973)
Supported by the Advanced Research Projects Agency under Contract HC-15-67-C-0221 and by AFOSR-71-2067

L. D. Yau and C. T. Sah
Quench-in Centers in Silicon p^+n Junctions
Solid State Electronics 17, 193-201 (1974)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GH-33634, and by AFOSR-71-2067

F. Hennig and C. T. Sah
Matrix Analysis of Distributed Semiconductor Circuit Models
Solid State Electronics 16, 1081-1083 (1973)
Supported by the National Science Foundation under Grant GK-30283

Sokrates T. Pantelides and C. T. Sah
Theory of Localized States in Semiconductors. I. New Results Using an Old Method
Physical Review (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GH-33634, and by AFOSR-71-2067

Sokrates T. Pantelides and C. T. Sah
Theory of Localized States in Semiconductors. II. The Pseudo Impurity Theory Application to Shallow and Deep Donors in Silicon
Physical Review (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GH-33634, and by AFOSR-71-2067

M. J. McNutt and C. T. Sah
The Effects of Spatially Inhomogeneous Oxide Charge Distribution on the MOS Capacitance-Voltage Characteristics
Journal of Applied Physics (submitted to)
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by the National Science Foundation under Grant GK-30283, and by AFOSR-71-2067

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Sokrates Theodore Pantelides (C. T. Sah, Adviser)
Theory of Point-Imperfection States in Semiconductors
June 1973
Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by AFOSR-71-2067, and by U. of I. Grad. Fellowship

Falke Hennig (C. T. Sah, Adviser)
Emission and Capture of Electrons and Holes at Gold Centers in Silicon at Thermal Equilibrium
May 1974
Supported by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by AFOSR-714-67, AFOSR-71-206, and by the National Science Foundation under Grants GH-33634 and GK-30283

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U. S. ATOMIC ENERGY COMMISSION

Interstitial Solid Solutions

Principal Investigator: Carl J. Altstetter, Sc.D.
Professor of Physical Metallurgy

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Carl J. Altstetter, Professor

Junior Staff: Dilip M. Shah, Research Assistant
Gary L. Steckel, Research Assistant
Peter F. Tortorelli, Research Assistant

Objectives: This program is concerned with the state of interstitial solute atoms in metals, their solubilities, the precipitates which form and their effect on properties. Effect of nitrogen solute and coherent nitride particles on mechanical behavior of vanadium is measured and correlated with the dislocation substructure, using electron microscopy.

Thermodynamic and kinetic measurements of oxygen solute in metals are carried out using solid electrolytic cells. Work on the effect of solute and precipitate structure on sputtering by energetic ion beams has begun. In all these studies particular attention has been given to the refractory metals and to obtaining the necessary understanding for their development for use in nuclear power production.

Approach: Measurement of the EMF of solid electrolytic cells, electron microscopy, tensile tests, ion beam bombardment.

Progress: (01 07 73 - 30 06 74) Thermodynamic properties of oxygen and oxide solubilities in niobium and tantalum have been determined with and without nitrogen in solution. Oxygen diffusion activation energies were determined in Nb and Ni. Vanadium-nitrogen alloy deformation experiments have been

completed, and the implications with regard to dispersion-hardening theory, until now developed in detail only for the face-centered cubic structure, are outlined. Study of the effect of solute and second phases on sputtering and damage due to energetic ions has begun. An ion beam apparatus for 0-30keV energies is being designed and built, including an UHV high temperature target chamber so that gas-metal interactions during bombardment can be investigated.

Publications: (01 07 73 - 30 06 74)

C. J. Altstetter and D. Hennessy
Influence of Austinite Stability on Fatigue of Stainless Steel
The Micro-Structure and Design of Alloys, Vol. 1, Institute of Metals, London, 1973, pp. 437-440
Supported by the U. S. Army Research Office

Carl Altstetter
Transformations in Rare Earth Metals
Metallurgical Transactions 4, 2723-2730 (1973)
Supported by the U. S. Army Research Office

William Nickerson and Carl Altstetter
A Thermodynamic Study of Niobium-Oxygen and Tantalum-Oxygen Solid Solutions Utilizing Solid Electrolytic Cells
Proceedings of the Third International Conference on Chemical Thermodynamics Baden, Vienna, 1973 (to be published)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Electronic Structure and Magnetism of Transition Metal Alloys

Principal Investigator: Paul A. Beck, M.S., M.E.
Professor of Physical Metallurgy

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Paul A. Beck, Professor

Junior Staff: Robert D. Shull, Research Assistant
Randal W. Tustison, Research Assistant

Objectives: Magnetic materials are technologically important in various applications, such as electric motors, generators, transformers and computer memory devices. The present project aims to contribute to a fuller fundamental understanding of magnetism in alloys of the 3d transition metals by studying (1) the effect of local atomic environment on the moment at 3d metal atoms, (2) the effect of magnetic clusters on the magnetic and transport properties of alloys.

Approach: Measurement of magnetic susceptibility, specific heat, electrical resistivity, and magnetoresistance.

Progress: (01 07 73 - 30 06 74) (a) The experimental study of magnetism of hcp Re-Co solid solution alloys has been completed. The results were presented at the Strasbourg International Conference on Disordered Alloys, Sept. 1973, and a brief report on this work will appear in the Proceedings of that Conference. Work is continuing on the interpretation of the results in terms of local spin fluctuations at Co sites with 8 and 9 Co nearest neighbors in combination with magnetic clusters comprising Co sites with 10 to 12 Co nearest neighbors.

(b) Study of the magnetic properties of Au-V alloys from 0.5% V to 20% V in the temperature range from 1.5° to 300°K. Ordered Au_4V has been described in the literature as ferromagnetic, but our preliminary results indicate that it may well be actually mictomagnetic instead. In the paramagnetic state the susceptibility of this alloy shows an unusual temperature dependence.

(c) The investigation of Cr-Fe and Cr-Fe-Al alloys has been completed. In addition to the Faraday method a low field ac method has also been used. The results prove the existence of mictomagnetism at concentrations between the Cr-rich antiferromagnetic and the ferromagnetic alloys at about 25 at.% Fe, and more. The giant moment and the concentration of the magnetic clusters was determined as a function of alloy composition and of temperature.

(d) Additional measurements are being made with Fe-Al alloys near the Fe_3Al composition, including some using the low-field ac method.

Publications: (01 07 73 - 30 06 74)

S. Mishra, E. J. Hayes, R. Tustison, and P. A. Beck
Magnetism in Ni-Cu and Co-Re Solid Solutions
Proceedings of the International Conference on Disordered Metallic Systems, Strasbourg, France, 1973, Journal de Physique 35, C4-194 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the National Science Foundation (Non-MRL)

S. Mishra and Paul A. Beck
Giant Moments in a Paramagnetic Copper-Nickel Alloy
International Journal of Magnetism 4, 277 (1973)
Supported by the National Science Foundation (Non-MRL)

S. Mishra and Paul A. Beck
Magnetic Properties of Cu-Fe Alloys
Physics Status Solidi 19a, 267 (1973)
Supported by the National Science Foundation (Non-MRL)

S. Mishra and Paul A. Beck
Magnetic Clusters in Dilute Alloys of Iron in Cu-Ni Solid Solutions
Physics Status Solidi 22a, (1974)
Supported by the National Science Foundation (Non-MRL)

S. Mishra
Magnetism in Cu-Ni Alloys
International Journal of Magnetism 5, 363 (1974)
Supported by the National Science Foundation (Non-MRL)

D. J. Chakrabarti
Effect of Atomic Ordering on the Magnetic Properties of Pd_3Mn and
of Some More Dilute Pd-Mn Alloys
International Journal of Magnetism (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

S. Mishra and P. A. Beck
Atomic Order-Disorder Information from Magnetic Data
Proceedings of the International Symposium on Order Disorder Transformations in Alloys, Tubingen, Germany, 1973 (to be published)
Supported by the National Science Foundation (Non-MRL)

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Anup Mukhopadhyay (Paul A. Beck, Adviser)
Magnetic Clusters in Mictomagnetic Cu-Mn Alloys
June 1974
Supported by the National Science Foundation (Non-MRL)

Point Defect - Dislocation Interactions

Principal Investigator: Howard K. Birnbaum, Ph.D.
Professor of Physical Metallurgy

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Howard K. Birnbaum, Professor
James R. Keiser, Research Associate

Junior Staff: Joseph J. Au, Research Assistant
Richard F. Mattas, Research Assistant (Term 4/20/74)
Philip E. Zapp, Research Assistant

Objectives: The diffusion of hydrogen and its isotopes in bcc metals is being studied from 4°K to 2500°K using magnetic and anelastic relaxation methods. Trapping effects at solutes and dislocations are being studied. The structure of complexes containing hydrogen and their role in determining hydrogen diffusivities is being investigated. The isotope effects in diffusion and in the interactions with trapping sites are being measured. This information is necessary for the intelligent utilization of bcc alloys (particularly refractory metal alloys) in environments containing H and its isotopes. Such applications are of increasing importance in energy generation and transportation systems.

Approach: Magnetic and anelastic relaxation techniques are used to study diffusion. Pure niobium crystals are prepared by electrolysis followed by high temperature removal of impurities and zone refining under very high vacuum conditions.

Progress: (01 07 73 - 30 06 74) The structure of the trapped O-H complex in Nb has been shown to consist of a <100> and a <111> defect and the binding

and motion enthalpy of each has been determined. The isotope effect on the defect relaxations and interactions have been measured. Similar results have been shown for the Fe-C-H and Fe-N-H system. This trapping has been shown to have a major effect on H diffusion at high temperatures.

Publications: (01 07 73 - 30 06 74)

C. Baker and H. K. Birnbaum
Anelastic Studies of Hydrogen Diffusion in Niobium
Acta Metallurgica 12, 865-872 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

J. J. Au and H. K. Birnbaum
Magnetic Relaxation Studies of Hydrogen in Iron: Relaxation Spectra
Scripta Metallurgica 7, 595-604 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

H. K. Birnbaum
Surface and Trapping Effects on Hydrogen Diffusion in bcc Metals
Scripta Metallurgica 7, 925-930 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

G. J. Sellers, A. C. Anderson, and H. K. Birnbaum
The Anomalous Heat Capacity of Superconducting Niobium
Physics Letters 44A, 173-174 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198
and by the National Science Foundation under Grant GH-33634

G. J. Sellers, A. C. Anderson, and H. K. Birnbaum
The Anomalous Heat Capacities of Niobium and Tantalum Below 1°K
Physical Review (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198
and by the National Science Foundation under Grant GH-33634

H. K. Birnbaum, M. Grossbeck, and S. Gahr
The Effects of Hydrogen on the Mechanical Properties and Fracture of Zr and Refractory Metals
A.S.M. Hydrogen Effects in Metals Book (in press)
Supported by the Office of Naval Research 00014-67-A-0305-0020

R. P. Walson and H. K. Birnbaum
Stress-Velocity Relations in High Purity Niobium
Physica Status Solidi (submitted to)
Supported by the Office of Naval Research 00014-67-A-0305-0020

R. P. Walson and H. K. Birnbaum
Dislocation Etch Pitting in High Purity Nb
Metallurgical Transactions (submitted to)
Supported by the Office of Naval Research 00014-67-A-0305-0020

M. S. Thesis: (01 07 73 - 30 06 74)

G. R. Holmquist (H. K. Birnbaum, Adviser)
Low Temperature Solubility of H in Nb
October 1973
Supported by the Office of Naval Research 00014-67-A-0305-0020

Ph.D. Thesis: (01 07 73 - 30 06 74)

R. F. Mattas (H. K. Birnbaum, Adviser)
Low Temperature Internal Friction in the Nb-H and Nb-O-H Systems
May 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

R. P. Walson (H. K. Birnbaum, Adviser)
Dislocation Velocity Measurements in High Purity Nb
January 1974
Supported by the Office of Naval Research 00014-67-A-0305-0020

Use of Very High Pressure to Investigate the Structure of Matter

Principal Investigator: Harry G. Drickamer, Ph.D.
Professor of Chemical Engineering and of Physical Chemistry
Member, Center for Advanced Study

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Harry G. Drickamer, Professor
Giovanni DePasquali, Research Assistant Professor
Nicholas Halasa, Research Associate (term 5/3/74)

Junior Staff: William D. Drotning, Research Assistant
Daniel L. Fanselow, Research Assistant (Term 6/6/74)
Eric N. Hockert, U.I. Fellow and Teaching Assistant
John Hook III, Research Assistant
Gary L. House, MMM Co. Research Assistant
Sang H. Moon, Research Assistant (Term 3/1/74)
Byron Okamoto, Research Assistant and Proctor Gamble Fellow
Craig E. Tyner, Shell Co. Foundation Fellow
Douglas G. Wilson, NSF-G Fellow
David L. Woracek, Research Assistant (Term 5/21/74)

Objectives: The purpose of this project is the investigation of the electronic behavior of solids, using very high pressure as a primary tool. Present experimental techniques permit optical absorption and luminescence measurements to 160 kilobars, electrical resistance studies to 500 kilobars, x-ray diffraction measurements to 400 kilobars, and Mössbauer resonance studies to 250 kilobars.

Our approach is to study the relative displacement of one set of orbitals with respect to another as pressure increases. From such studies we can evaluate the parameters describing the ground state and excited state potential wells. Under many circumstances we observe an electronic transition to a new ground state whose properties we can also evaluate.

Projects currently active include studies of bonding and magnetism in ferrites, studies of photochromism, thermochromism and piezochromism, the characterization of excited states from high pressure absorption and fluorescence measurements, and luminescence studies on a wide variety of inorganic and organic phosphors.

Approach: Optical absorption, luminescence, electrical resistance, x-ray diffraction, and Mössbauer measurements as a function of pressure.

Progress: (01 07 73 - 30 06 74) (1) We have developed techniques for studying photochromism and thermochromism to 150 kilobars. (2) We have developed techniques for making solid state luminescent measurements to 150 kilobars. (3) We have extended the 12 kbar liquid fluorescence capabilities to include lifetimes as well as peak shifts and intensities. (4) We have demonstrated the ability to characterize in detail electronic parameters from high pressure absorption and emission studies and applied the techniques to anthracene and phenanthrene. (5) We have initiated fluorescence studies on heavy metal doped alkali halides. (6) We have characterized pressure effects on orthoferrites, Fe_3O_4, and $NiFe_2O_4$.

Publications: (01 07 73 - 30 06 74)

H. G. Drickamer
High Pressure, Electronic Structure, and Chemistry in Solids
Chemistry in Britian 9, 353-359 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

P. J. Wang and H. G. Drickamer
High Pressure Optical Studies of Rare Earth Ions in CaF_2 and other Fluorides
Journal of Chemical Physics 58, 4444-4446 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

P. J. Wang and H. G. Drickamer
The Reduction of Cu(II) at High Pressure
Journal of Chemical Physics 59, 713-717 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

P. J. Wang and H. G. Drickamer
Transformation from Tetrahedral to Planar Symmetry in Cs_2CuCl_4 and Cs_2CuBr_4 at High Pressure
Journal of Chemical Physics 59, 559-560 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

V. C. K. Chiu and H. G. Drickamer
High Pressure Spectral Studies of Mixed Valence Compounds of Antimony
Proceedings of the National Academy of Sciences 70, 3065-3066 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

W. D. Drotning and H. G. Drickamer
The Effect of Pressure on the Optical Absorption of REF Centers in Ce and Tb Doped CaF_2
Journal of Chemical Physics 59, 3482-3484 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

H. G. Drickamer
Electronic Transitions in Transition Metal Compounds at High Pressure
Angewandte Chemie 13, 39-47 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

N. A. Halasa, G. DePasquali, and H. G. Drickamer
High Pressure Studies on Ferrites
Physical Review (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Gregorio Weber, Fumio Tanaka, Byron Y. Okamoto, and H. G. Drickamer
The Effect of Pressure on the Molecular Complex of Isoalloxazine and Adenine
Proceedings of the National Academy of Sciences (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

B. Y. Okamoto, W. D. Drotning, and H. G. Drickamer
The Evaluation of Configuration Coordinate Parameters from High Pressure Absorption and Luminescence Data
Proceedings of National Academy of Sciences (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

S. H. Moon and H. G. Drickamer
The Effect of Pressure on Hydrogen Bonds in Organic Solids
Chemical Physics (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

B. Y. Okamoto and H. G. Drickamer
The Evaluation of Configuration Coordinate Parameters from High Pressure Optical Data I: Phenanthrene, Anthracene, and Tetracene
Journal of Chemical Physics (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

B. Y. Okamoto and H. G. Drickamer
The Evaluation of Configuration Coordinate Parameters from High Pressure Optical Data II: Purine and Pyrimidine Bases and Nucleosides
Journal of Chemical Physics (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

D. L. Fanselow and H. G. Drickamer
High Pressure Studies of the Elevytonic Behavior of Bianthrones
Journal of Chemical Physics (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

Douglas Wilson (H. G. Drickamer, Adviser)
High Pressure Studies of Anthracene Homologues
June 1973
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

D. L. Woracek (H. G. Drickamer, Adviser)
Effects of Pressure on Alkali Halides Doped with Lead (II)
June 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Ph.D. Thesis: (01 07 73 - 30 06 74)

V. C. K. Chiu (H. G. Drickamer, Adviser)
High Pressure Studies on Mixed Valence Systems
October 1973
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Nicholas Allen Halasa (H. G. Drickamer, Adviser)
Hyperfine Interactions in Ferrites and Orthoferrites at High Pressure
February 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Sang Heup Moon (H. G. Drickamer, Adviser)
High Pressure Studies on Hydrogen Bonding in Solids
May 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Deformation of Intermetallic Compounds at Elevated Temperatures, and an Assessment of the Capabilities of the Scanning Transmission Electron Microscopy Unit

Principal Investigator: Hamish L. Fraser, Ph.D.
Assistant Professor of Metallurgy

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Hamish L. Fraser, Assistant Professor
Ian Philip Jones, Visiting Research Professor (9/21-11/20/73)

Junior Staff: Nestor J. Zaluzec, Research Assistant
Robert Abbott, Industrial Student

Objectives: The object of the research program falls into two sections. Firstly, the work is aimed at understanding the elevated temperature mechanical properties of intermetallic compounds. At present the work is concerned with investigating two areas of the plastic deformation of simple crystals which are not understood, namely kinking and uniform deformation which occurs when simple crystals of NiAl (for example) are compressed along <100> directions. In the former case, a theory of kinking has been developed by the author, and the work on this phenomenon now consists of a series of experiments to substantiate that theory. In the latter case, the work is concerned with determining the rate of climb in intermetallic compounds since it appears from preliminary work that climb may be responsible for plastic deformation at elevated temperatures. Combined transmission electron microscopy, measurements of lattice rotations and strain rate tests are being carried out.

An assessment of the capabilities of the scanning transmission electron microscopy unit is currently being carried out. In particular, a comparison of the useful electron penetration is being determined by means of a controlled experiment involving thin films of gold.

Approach: Electron microscopy, electron diffraction, and strain rate determinations.

Progress: (01 07 73 - 30 06 74) During this period, three advances have been made. Firstly, the theory for kinking developed in earlier work has been used to predict kinking in some crystal structures where this type of determination has not yet been observed. Experiments of LiF and CaF_2 are in progress to substantiate this prediction. Secondly, progress towards the determination of the rate of climb in the elevated temperature deformation of NiAl has been made. We have observed for compression along <100> directions at 1000°K: a) no crystal rotations as a result of compression: b) no observable slip lines; c) dislocations of the type $\underline{b}$ = <100>, as expected: d) dislocations of the type $\underline{b}$ = <110> usually contained in networks; e) crystallographic analysis reveals that the dislocation of $\underline{b}$ = <110> are probably not slip dislocations. These observations are entirely consistent with climb acting as the major mechanism for plastic strain.

Finally, work on assessing the STEM unit has commenced and so far some progress involving the thickness dependence of resolution has been made. Dislocation image widths of 60-70 Å have been measured, even at the point where the foil is too thick for acceptable contrast to be obtained.

Publications: (01 07 73 - 30 06 74)

H. L. Fraser, N. H. Loretto, and R. E. Smallman
Direct Observations of the Annealing of Stacking-Fault Tetrahedra in Gold Using High Voltage Electron Microscopy
Philosophical Magazine 28, 1043 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Anharmonic Effect in Solids

Principal Investigator: Andrew V. Granato, Ph.D.
Professor of Physics

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Andrew V. Granato, Professor
Ricardo B. Schwarz, Research Associate

Junior Staff: Terrell D. Berker, Research Assistant
Randall D. Isaac, Research Assistant
David T. Read, Research Assistant

Objectives: We have been engaged in a program of understanding the non-linear elastic properties of materials of systematically increasing complexity. We propose now to use results previously found for materials of different bonding types and crystal structures in applications to studies of thermal properties, phase transitions, and defects in crystals.

Approach: Ultrasonic transmission and absorption techniques.

Progress: (01 07 73 - 30 06 74) (1) Third order elastic constants have been used to describe the thermodynamic properties of the martensitic hexagonal close packed to face centered cubic transition of a cobalt-nickel alloy. (2) Experimental evidence has been obtained for (a) the <100> split configuration of free interstitials, (b) resonance modes of free interstitials, and (c) the configuration of the Stage I_c close-pair defect in copper.

Publications: (01 07 73 - 30 06 74)

E. R. Fuller, Jr., A. V. Granato, J. Holder, and E. R. Naimon
Ultrasonic Studies of the Properties of Solids
Methods of Experimental Physics, Ed. by R. V. Coleman (1974) pp. 371
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198, by the National Science Foundation under Grant GP-27369, and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221

A. V. Granato
Microscopic Mechanisms of Dislocation Drag
Metallurgical Effects at High Strain-Rates, Ed. by R. W. Rhode, et. al., Plenum Press (1973), pp. 255
Supported by the National Science Foundation under Grant GH-27369

E. R. Fuller, Jr. and W. F. Weston
Relation Between Elastic-Constant Tensors of Hexagonal and Cubic Structures
Journal of Applied Physics (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

L. E. Rehn, J. Holder, A. V. Granato, R. R. Coltman, and F. W. Young, Jr.
Effects of Thermal Neutron Irradiation on the Elastic Constants of Copper
Physical Review Letters (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and the National Science Foundation under Grant GH-33634

J. Holder, A. V. Granato, and L. E. Rehn
Effects of Interstitials and Close Pairs on Elastic Constants
Physical Review Letters (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the National Science Foundation under Grant GH-33634

J. Holder, A. V. Granato, and L. E. Rehn
Experimental Evidence for Split Interstitials in Copper
Physical Review Letters (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the National Science Foundation under Grant GH-33634

A. V. Granato
Effects of Dislocation Interactions with Electrons and Phonons
Proceedings of the Fifth International Conference on Internal Friction and Ultrasonic Attenuation in Crystalline Solids, Ed. by K. Lüchi, Springer-Verlag (to be published)
Supported by the National Science Foundation under Grant GH-37907

A. V. Granato and R. W. Balluffi
Dislocations, Vacancies, and Interstitials
Treatise on Dislocation Theory, Ed. by F. R. N. Navarro, Dekker (to be published)
Supported by the National Science Foundation under Grant GH-37907

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Lynn Eduard Rehn (J. T. Holder and A. V. Granato, Advisers)
Contributions from Point Defects to the Elastic Constants of Copper
February 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198
and by the National Science Foundation under Grant GH-33634

Radiation Damage in Solids

Principal Investigator: James S. Koehler, Ph.D.
Professor of Physics

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: James S. Koehler, Professor
Wolfram Hertz, Research Associate

Junior Staff: Noel K. Barbulesco, Research Assistant
James R. Bethin, Research Assistant (Term 5/20/74)
Robert C. Birtcher, Research Assistant

Objectives: We are attempting to determine the geometrical structure and the physical properties associated with point defects in metals and in semiconductors.

Approach: 3MEV electron beam irradiation of semiconductors and metals, electrical resistance measurements, observation of proton channeling in single crystals.

Progress: (01 07 73 - 30 06 74) (1) Dr. R. Roop measured changes in ac hopping conductivity of P type germanium during electron irradiation at 1.7°K. Result: A defect migrates during electron irradiation at 1.7°K in P type germanium. (2) Dr. Y. Lwin, R. Birtcher, and E. Ryan irradiated lead at 3°K. In contrast with earlier research 50% of the damage introduced anneals below 8°K. Various annealing steps are observed.

Publications: (01 07 73 - 30 06 74)

P. S. Gwozdz and J. S. Koehler
Electron Irradiation of Gold Below 2 K
Physical Review B8, 3616-3627 (1973)
Supported by the U. S. Army Research Office (Durham)

J. S. Koehler
Point Defects in Metals
Proceedings of Conference on Point Defects, Tbilissi, USSR, 1973
(to be published)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

J. S. Koehler
Point Defects in Semiconductors
Proceedings of Conference on Point Defects, Tbilissi, USSR, 1973
(to be published)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Raymond Mervin Roop (J. S. Koehler, Adviser)
Effects of Electron Irradiation on P-Type Germanium at Liquid Helium Temperatures Using AC Hopping Conductivity
October 1973
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the U. S. Army Research Office (Durham)

Defect and Electronic Properties of Solids

Principal Investigator: David Lazarus, Ph.D.
Professor of Physics

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: David Lazarus, Professor
John P. Bensel, Research Associate

Junior Staff: Paul C. Allen, Research Assistant
Richard S. Hockett, Research Assistant (Term 5/29/74)
Mark S. Jackson, Research Assistant
Joan L. Mitchell, Research Assistant
Jonathon D. Weiss, Research Assistant (Term 9/30/73)

Objectives: Experimental and theoretical studies are undertaken to investigate the defect and electronic properties of classic prototype solids as a function of hydrostatic pressure and temperature to determine the basic atomic mechanisms which enter into mass, charge, and thermal transport in a wide variety of materials. Particular emphasis is placed on studies of diffusion mechanisms, thermoelectric properties, and fluctuations in electrical noise near phase transitions.

Approach: Thermoelectric power measurements as a function of pressure and temperature. Radioactive tracer diffusion measurements. Measurement of electronic noise.

Progress: (01 07 73 - 30 06 74) Work was completed on a study of the effect of hydrostatic pressure on the helium-temperature thermoelectric power of sodium, indicating scaling consistent with Bailyn's model for the phonon drag region. Tracer diffusion studies have been conducted on alkali halide crystals with surface tracer divalent impurities, with results consistent with the earlier theoretical model. Measurements have been completed on

the effect of pressure on the high-temperature thermoelectric power of chromel-alumel and platinum-rhodium thermocouples. A study to detect a new type of "magneto-flicker" noise in potassium, predicted by Overhouser as resulting from charge density waves, showed no effect within limits of several orders of magnitude below the predicted value. Work has been started on building up a broad-spectrum noise measuring capability and on a measurement of the isotope effect for tin isotopes diffusing in titanium.

Publications: (01 07 73 - 30 06 74)

Georges Martin, David Lazarus, and Joan Mitchell
Pressure Dependence of Self-Diffusion of Na^{22} in NaCl
Physical Review B8, 1726-1731 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Michael D. Feit, Joan Mitchell, and David Lazarus
Effect of Surface Impurities on Tracer Diffusion in Insulators
Physical Review B8, 1715-1725 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

V. M. Cheng, R. K. Crawford, and W. B. Daniels
Molar Volume of Argon Along the Melting Curve up to 10 kbar
Physics Letters 43A, 109-110 (1973)
Supported by the U. S. Atomic Energy Commission under Contract At(11-1)-1198, and by the National Science Foundation under Grant GP-7739 and GP-18573 (Princeton)

David Lazarus and Joan L. Mitchell
Effect of Surface Impurities on Tracer Diffusion in Ionic Crystals
International Conference on Lattice Defects in Ionic Crystals, Marseille, France, 1973 (to be published)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Jonathon D. Weiss and D. Lazarus
Pressure Dependence of the Thermoelectric Power of Sodium Between 5°K and 14°K
Physical Review B (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Jonathan David Weiss (D. Lazarus, Adviser)
The Pressure Dependence of the Thermoelectric Power of Sodium Between 5°K and 14°K
February 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Deformation of Reinforced Metals

Principal Investigator: Marvin Metzger, Ph.D.
Professor of Physical Metallurgy

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Marvin Metzger, Professor

Junior Staff: Prabir R. Bhowal, Research Assistant

Objectives: To develop realistic models of matrix behavior at small strains in composite crystalline materials and provide information applicable to the design of technological materials containing nondeforming phases. Our previous model system, W-Cu, appeared to involve difficulties for substantial extension of our previous work, and we have begun work on Ni_3Al-Ni_3Nb aligned eutectic alloys, in which the desired situation of a closely and variably spaced reinforcing phase is experimentally accessible.

Approach: Microstrain measurements and electron microscopy.

Progress: (01 07 73 - 30 06 74) In this period, we expect to refine specimen handling techniques for our alloy and to make some of the microyielding and macroyielding tests together with some of the electron microscope observations of dislocation structure which will guide subsequent efforts.

Publications: (01 07 73 - 30 06 74)

J. Zahavi and M. Metzger
Effect of Chloride on Growth of an Anodic Film
Journal of the Electrochemical Society 121, 268-279 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the U. S. Army Research Office (Durham)

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

The Mechanism of Stress-Corrosion Cracking: Propagation Studies

Principal Investigator: E. Neville Pugh, Ph.D.
Professor of Metallurgical Engineering

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: E. Neville Pugh, Professor

Junior Staff: Gerhardus H. Koch, Research Assistant
J. Lawrence Nelson, Research Assistant

Objectives: A major barrier to progress in understanding the mechanisms of stress-corrosion cracking (SCC) of alloys in aqueous media is lack of knowledge concerning the crack-propagation process--in particular, is cracking continuous or discontinuous? The immediate object of the present work is to answer this critical and controversial question. Results obtained during the pursuit of this objective have strongly suggested that failures in several important alloy systems results from the entry of cathodically-generated hydrogen into the metal lattices, and thus a second objective is to investigate this possibility.

Approach: Optical and electron microscopic examination of fracture surfaces and acoustic emission observations during fracture.

Progress: (01 07 73 - 30 06 74) Detailed fractographic and acoustic-emission studies have shown that the transgranular SCC of a single-phase Mg-Al alloy in aqueous chloride-chromate solutions, thought by many workers to involve continuous anodic dissolution, in fact occurs by discontinuous cleavage on $\{31\bar{4}0\}$, and that failure is due to hydrogen. The latter view gained strong support from our observation that a closely similar failure occurs in dry gaseous hydrogen. The crack-propogation studies have been extended

to the transgranular SCC of alpha-phase Ti-Al (also HCP) in aqueous chlorides, and results to date indicate that the characteristics are the same as the Mg-Al case.

Publications: (01 07 73 - 30 06 74)

None

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Nuclear Magnetic Resonance Studies

Principal Investigator: Theodore J. Rowland, Ph.D.
Professor of Physical Metallurgy

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Theodore J. Rowland, Professor

Junior Staff: Lance C. Labun, Research Assistant
Robert S. Shalvoy, Research Assistant
Andrew C. Yen, Research Assistant (Term 3/21/74)

Objectives: This project, consistent with its rather broad title, aims at both specific and exploratory investigations. The latter are concentrated in the area of potential applications of nuclear magnetic resonance to phenomena of practical metallurgical-materials interest. It is thus partially aimed at considering and developing the usefulness of the technique as a tool. In this latter class of studies fall various studies on concentrated alloys, order-disorder transformations, diffusion and precipitation.

Approach: Nuclear magnetic resonance techniques and field ion microscope observation.

Progress: (01 07 73 - 30 06 74) The age hardening process of a Cu -2 wt.% Be alloy was examined by resonance intensity measurements supplemented by field-ion microscopy. The results provide evidence of lattice strain and solute concentration in the matrix surrounding this very fine (CuBe) precipitate even in "over-aged" alloys. The matrix solute concentration is found to be in excess of the value quoted on the published phase diagram, but in keeping with the applicable thermodynamic considerations (Thomson-Freundlich equation).

Work on the diffusion of hydrogen in niobium has progressed: samples were prepared and some data obtained. A technique is being investigated which has the required sensitivity to study the dilute solid solutions of interest and some advance in interpretation of the data in terms of nuclear relaxation time has been made.

Equipment has been constructed and some measurements made extending our work on elastomers. One rubber sample exhibited a ten percent increase in relaxation time when close to elastic limit. Much more closely controlled experiments on vulcanized polybutadiene have begun.

Publications: (01 07 73 - 30 06 74)

None

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Andrew Chien-Chong Yen (T. J. Rowland, Adviser)
A Study of Precipitation in Copper +13 Atomic Percent Beryllium by Nuclear Magnetic Resonance and Field Ion Microscopy
June 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Properties of Noble Gas Crystals

Principal Investigator: Ralph O. Simmons, Ph.D.
Professor of Physics;
Head, Department of Physics

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Ralph O. Simmons, Professor
Roy K. Crawford, Assistant Professor

Junior Staff: Duane R. Aadsen, Research Assistant
William H. Hardy, Research Assistant (Term 11/16/73)
Steve M. Heald, Research Assistant
Albert T. Macrander, Research Assistant (Term 1/5/74)
Mark P. Zaitlin, Research Assistant and NSF-G Fellow

Objectives: Study of defect structure and lattice dynamics of noble gas and other molecular crystals. Noble gas crystals are model substances for testing theoretical ideas about defect formation and mobility and about lattice dynamics, when the interatomic interactions are fairly well defined also from data on the liquid and gaseous phases. In crystalline helium such effects can be studied over a broad range of densities. Defect characteristics are probed by x-ray scattering, macroscopic observation, and by optical scattering. Crystalline methanes offer the opportunity to study many phase transitions systematically.

Approach: X-ray diffraction and laser Raman light scattering techniques. Measurement of thermal coefficient of expansion.

Progress: (01 07 73 - 30 06 74) 1) A comprehensive set of measured structure factors for Si were compared to LCMBF calculations and the temperature dependences of selected Bragg diffraction peaks were compared to existing

models of phonon frequency spectra in Si. 2) A model of the vacancy in Ne was studied via an extended Hückel scheme. 3) Thermal expansion of the fcc substances Ar, Kr, Al, Cu, Ag, Au, and Pb was compared in the high-temperature region to models of the Swenson and of the Choquard type. 4) Construction of a new x-ray diffraction cryostat for T>50 mK was completed and bcc ^{3}He work carried to lower temperatures. 5) X-ray studies of CH_4 and CD_4 were completed for the high T phase. 6) Raman scattering from solid Ar up to 7 kbar was begun.

Publications: (01 07 73 - 30 06 74)

R. Balzer and R. O. Simmons
Thermal Defects in bcc ^{3}He Crystals Determined by X-ray Diffraction
Proceedings Thirteenth International Conference on Low Temperature Physics LT13, Vol. II, pp. 115-119 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

R. K. Crawford
Hard Sphere Melting Model: Melting in Argon
Journal of Chemical Physics 60, 2169-2174 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

R. K. Crawford
Melting, Vaporizations, and Sublimation
Rare Gas Solids, edited by M. L. Klein and J. A. Venables (Academic Press, New York, 1974) Vol. 1
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

L. A. Schwalbe
Equilibrium Vacancy Concentration Measurements in Solid Argon
Physical Review (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

William Harold Hardy II (R. O. Simmons, Adviser)
Debye-Waller Measurements in Silicon
May 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Nuclear Magnetic Resonance in Solids

Principal Investigator: Charles P. Slichter, Ph.D.
Professor of Physics
Member, Center for Advanced Study

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Charles P. Slichter, Professor
Stephen Meyer, Research Associate

Junior Staff: Thomas J. Aton, Research Assistant and IBM Fellow
John V. Crues, Research Assistant (Term 5/20/74)
David M. Follstaedt, Research Assistant
James P. Long, Research Assistant
Thomas S. Stakelon, Research Assistant
Lawrence R. Whalley, Research Assistant (Term 1/5/74)

Objectives: (1) Study the Dilute Magnetic Systems - Kondo Effect. One of the basic problems of solid state physics is the circumstances under which magnetism occurs. For this reason there is great theoretical and experimental interest in systems of dilute amounts of transition metal atoms (such as Fe) which one conventionally thinks of as magnetic in nonmagnetic host metals (such as Cu, Al, or Ag). The interesting feature of such systems is that under some circumstances (e.g. Mn and Fe in Cu at room temperature) the "magnetic atom" acts magnetic, but in other cases (e.g., in Mn in Al at room temperature or Fe in Cu at helium temperatures) it is nonmagnetic.

As a starting point, theoretical treatments distinguish between two regimes, magnetic and non-magnetic. However, the coupling of the magnetic system to the conduction electrons must be treated as a true many-body problem below a certain temperature called the Kondo temperature, T_K, leading to the system appearing non-magnetic below T_K. The phenomena is called the Kondo effect.

The question arises, can one distinguish a conventional non-magnetic system from a magnetic system below its Kondo temperature?

We are investigating this and other questions concerning the electronic state of magnetic atoms in non-magnetic hosts.

The experimental technique is to probe the electronic wave function of the conduction electrons in the near vicinity of the impurity through nuclear resonance and nuclear double resonance of the near neighbors. Crudely speaking, we measure the energy dependence of the magnetic scattering of the conduction electrons from the impurity, probing for the location and width of spin-dependent scattering resonances.

(2) Layer compounds, of which TaS_2 is an example, exhibit many interesting properties including strong effects on the superconducting transition temperature when various molecules are intercalated. We have been joined by a recent Ph.D., Dr. Stephen F. Meyer, who has worked on the TaS_2 system at Stanford with Professor T. Geballe. We are carrying out magnetic resonance studies of these systems to try to gain insight into the role of the intercalated molecules.

(3) Pressure Induced Chemical Changes. Slichter is continuing the collaboration with Professor Drickamer of the Department of Chemistry on the theory of Professor Drickamer's high pressure experiments. The current work is relating the changes in optical spectra to the changes in Mössbauer spectra, expecially using the optical spectra to show that pressure has caused a new electronic state to become the ground state.

Approach: Nuclear and electron spin resonance techniques.

Progress: (01 07 73 - 30 06 74) (1) We have found resonance due to Cu atoms which are neighbors to V, Cr, Mn, and Fe, so-called "satellite lines". (2) We have studied their field and temperature dependences. We have followed the satellites in CuFe from above to below the 29K Kondo temperature, showing that there is no change in the shape of the spin polarization as one passes through the Kondo temperature, contrary to some theories. (3) We have found satellites in single crystals of CuCo and CuNi, and have started work on CuFe single crystals. (4) We have completed NMR studies of K and Cs but find no signs of the charge density oscillations predicted by Overhauser. (5) We have continued the collaboration of interpretation of Professor Drickamer's pressure studies.

Publications: (01 07 73 - 30 06 74)

David Lo, David V. Lang, James B. Boyce, and Charles P. Slichter
NMR Studies of Dilute Alloys of Ni in Cu
Physical Review B8, 973-979 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

W. J. Meyer, D. V. Lang, and C. P. Slichter
Electric Field Nuclear Double Resonance in Ag^+ Doped NaCl
Physical Review B8, 1924-1934 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

David V. Lang, David C. Lo, James B. Boyce, and C. P. Slichter
Measurements of Electron Spin Density Near Co Atoms in Cu
Physical Review B9, 3077-3085 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

James B. Boyce and Charles P. Slichter
The Conduction Electron Spin Density Around Fe Impurities in Cu Above and Below T_K
Physical Review Letters 32, 61-64 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Lawrence R. Whalley and Charles P. Slichter
Electric Field Gradients in Copper-Nickel Alloys
Physical Review (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

James B. Boyce, Thomas Aton, Thomas Stakelon, and Charles P. Slichter
Spin Polarization Near Iron Group Atoms in Cu
Journal of Pure and Applied Chemistry (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Charles P. Slichter
Some Scientific Contributions of Herbert S. Gutowsky
Journal of Pure and Applied Chemistry (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Lawrence Robert Whalley (C. P. Slichter, Adviser)
Electric Field Gradients in Copper Alloys
February 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Solid State Phase Transformations and Thin Films

Principal Investigator: C. Marvin Wayman, Ph.D.
Professor of Metallurgical Engineering

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: C. Marvin Wayman, Professor
Hua-Ching Tong, Research Assistant Professor (Term 3/31/74)

Junior Staff: Gilles P. Asselin, Research Assistant (Term 2/10/74)
Yue-Kong Au, Research Assistant
Michael P. Cassidy, Research Assistant (Begin 2/21/74)
S. Chakravorty, Research Assistant
Terry Alan Schroeder, Research Assistant (Term 2/21/74)

Objectives: Phase transformations in thin films and bulk materials are studied. Emphasis is on pretransformation lattice oscillations, as observed in thin films (electron microscopy and diffraction); characteristics and properties of metallic hydride formation: crystallography and features of martensite formation in NiAl alloys: nucleation, growth and substructure of phases formed in sputtered alloy thin films; the amorphous-to-crystalline transformation in Ga-Sb and In-Sb alloys; thermoelastic martensitic transformations; and feasibility of metallic energy conversion devices based on the martensitic transformation and shape memory effect.

Approach: Electron microscope observations and electron diffraction measurements. Preparation of thin films by vacuum evaporation and sputtering.

Progress: (01 07 73 - 30 06 74) Significant accomplishments have been made in identifying pretransformation effects by electron microscopy and diffraction. Precursory events, definitely related to martensitic transformations in a number of alloys, have been seen by studying thin films. Such observations

lead directly into theoretical and experimental work on thermoelastic martensitic transformations has established two characteristic temperatures (T_o and T_o') which establish regimes for the balance between chemical and nonchemical free energies. The effect of parent phase ordering in favoring a thermoelastic martensitic transformation has been explained on the basis of differences in bonding enthalpies. Studies of martensitic transformations in sputtered alloy films, hydrogen charged materials, and NiAl alloys have been initiated. Investigations of the nucleation and growth of certain fcc and bcc metals evaporated on various substrates have been concluded.

Publications: (01 07 73 - 30 06 74)

I. Cornelis and C. M. Wayman
Phase Transformations in Metastable β' CuZn Alloys I:
Martensitic Transformations
Acta Metallurgica 22, 291-300 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

I. Cornelis and C. M. Wayman
Phase Transformations in Metastable β' CuZn Alloys II:
Isothermal Transformations
Acta Metallurgica 22, 301-311 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

H. C. Tong and C. M. Wayman
Some Stress-Temperature-Energy Relationships for Thermoelastic
Martensitic Transformations
Scripta Metallurgica 8, 93-100 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

I. Cornelis, R. Oshima, H. C. Tong, and C. M. Wayman
Direct Observations of Pretransformation Lattice Instabilities
Scripta Metallurgica 8, 133-144 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

C. M. Wayman
Phase Transformations in 'Less Common' Materials
Metallurgical Transactions 4, 2781-2787 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198, by the National Science Foundation under Grant GH-36813, and by the U. S. Army Research Office

H. C. Tong and C. M. Wayman
Direct Evidence of Pretransformation Lattice Instabilities
Physical Review Letters (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

H. C. Tong and C. M. Wayman
Characteristic Temperatures and Other Properties of Thermoelastic Martensites
Acta Metallurgica (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198, and by the National Science Foundation

H. C. Tong and C. M. Wayman
A Simplified Calorimeter for Determining Latent Heats of Martensitic Transformations at Low Temperatures
Metallurgica Transactions (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198, and by the U. S. Army Research Office (Durham)

H. C. Tong and C. M. Wayman
Thermodynamics of Thermoelastic Martensitic Transformations
Acta Metallurgica (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the U. S. Army Research Office (Durham)

M. S. Thesis: (01 07 73 - 30 06 74)

Terrence Alan Schroeder (C. M. Wayman, Adviser)
Shape Memory Behavior and Mechanical Characteristics of Some Copper Zinc Alloys
June 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the National Science Foundation under Grant GH-36813

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Precipitation in Refractory Metal Alloys

Principal Investigator: Charles A. Wert, Ph.D.
Professor of Physical Metallurgy;
Head, Department of Metallurgy and Mining Engineering

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Charles A. Wert, Professor
Edwin L. Pollock, IBM Postdoc Fellow

Junior Staff: Christian P. Fluhr, Research Assistant (Term 5/20/74)
Philippe L. Lecocq, Research Assistant (Term 4/12/74)
Robert W. Levis, Research Assistant (Begin 4/13/74)

Objectives: This work has the goal of determining the behavior of V, Nb and Ta and some of their alloys in environments of hydrogen and oxygen. In particular the role of oxygen dissolved in the metals in trapping hydrogen will be investigated. The nature of the strengthening caused by dispersions of carbides in these alloys will also be examined.

Approach: Measurement of gas solubility, transmission and scanning electron microscopy.

Progress: (01 07 73 - 30 06 74) a) We have quantitatively determined the solubility of hydrogen and deuterium in Ta. We have also looked qualitatively at the kinetics of hydride formation. b) We have examined precipitates of carbides in alloys of V with Ti in an attempt to produce dispersion of coherent carbides stable to temperatures well over half the melting point.

Publications: (01 07 73 - 30 06 74)

H. Y. Chang and C. A. Wert
The Solubility and Trapping of Hydrogen in Vanadium
Acta Metallurgica 21, 1233-1242 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

O. Buck, D. O. Thompson, and C. A. Wert
An Explanation for the α-Peak in Hydrogenated Niobium
Journal of Physics and Chemistry of Solids 34, 591-595 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

B. Ganguly, C. Wert, and J. Woodhouse
Microchemistry of Copper-Infiltered Iron Powder
International Journal of Powder Metallurgy 10, 87-99 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

J. B. Woodhouse, A. L. A. Fields, and I. A. Bucklow
X-ray Mass Absorption Coefficients for Gold, Lead, and Bismuth in the Range 1 Å to 10 Å
Journal of Physics D: Applied Physics 7, 483-489 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

R. K. Viswanadham and C. A. Wert
Precipitation from Supersaturated Nb-C Solid Solutions
Metallurgical Transactions 5, 123-126 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

H. Y. Chang and C. A. Wert
The α-Peak in Vanadium
Proceedings of Conference on Internal Friction and Ultrasonic Attenuation in Crystalline Solids, Aachen, Germany, 1973 (to be published)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

H. Y. Chang and C. A. Wert
Precipitation of Carbides in Deformed Vanadium
Metallurgical Transactions (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

H. Y. Chang, R. K. Viswanadham, and C. A. Wert
Age Hardening in the V-C and Nb-C Systems
Metallurgical Transactions (submitted to)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

Christian Paul Fluhr (C. A. Wert, Adviser)
An Electron Microscopy Study of Carbide Precipitation in a Vanadium-Titanium Alloy
May 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Ph.D. Thesis: (01 07 73 - 30 06 74)

None

Physics of Refractory Materials

Principal Investigator: Wendell S. Williams, Ph.D.
Professor of Physics, of Ceramic Engineering,
and of Bioengineering

Supporting Agency: U. S. Atomic Energy Commission

Senior Staff: Wendell S. Williams, Professor

Junior Staff: Joseph G. Baldoni, Research Assistant
Lance Breger, University Assistant
Alvin P. Gerk, Graduate Student (Term 10/23/73)
Marvin W. Johnson, Research Assistant
Michael Kolber, Teaching Assistant
Subhash Kulkarni, Research Assistant
Daniel Petty, Research Assistant

Objectives: The program centers on the determination and interpretation of thermal, mechanical and electrical properties of the transition metal carbides, a class of materials exhibiting extreme values of these properties. Recently the program has expanded to include a study of the physical properties of hard natural tissues, the apatite-bearing materials, bone and teeth.

Approach: Tensile tests, ultrasonic internal friction measurements, Lang x-ray topography, scanning electron microscopy, and piezoelectric measurements.

Progress: (01 07 73 - 30 06 74) A systematic investigation of the internal friction of Ge and Si at high temperatures was completed. The damping of 150 KHz waves was shown to be severe and dislocation-related. A theoretical model which satisfactorily interpreted the data was developed: the model is based on electronic viscous damping of dislocations by excess current carriers whose lifetimes are controlled by Auger recombination processes. A qualitative way of thinking about the strong bonding in the carbides was proposed: the total cohesive energy is the sum of a large metal-metal d-band interaction which is little changed when the compound is formed; additional

covalent bonding between metal and carbon atoms is introduced on compound formation, but at the expense of breaking the strong carbon-carbon bond in graphite: a small additional contribution to the cohesive energy comes from the partially ionic character of the carbide--this contribution is equal to the heat of formation. Measurements of the piezoelectric response of tendon and bone in cantilever bending showed signals as large as a volt. The standard theory of piezoelectricity had to be extended to include a contribution to the polarization from the gradient of the stress, via a 4th rank tensor. Predictions from this formal theory were tested in the laboratory and found to be correct. Scanning electron micrographs of etched surfaces of tooth enamel revealed clearly the characteristic enamel prisms and their matrix.

Publications: (01 07 73 - 30 06 74)

L. W. Shacklett and Wendell S. Williams
Influence of Order-Disorder Transformations on the Electrical Resistivity of Vanadium Carbide
Physical Review B7, 5041-5053 (1973)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

Wendell S. Williams
Sources of Piezoelectricity in Tendon and Bone
Critical Reviews in Bioengineering 2, 95-118 (1974)
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

M. S. Thesis: (01 07 73 - 30 06 74)

None

Ph.D. Thesis: (01 07 73 - 30 06 74)

Alvin Phillip Gerk (W. S. Williams, Adviser)
Friction in Intrinsic and N-Type Germanium and Silicon
February 1974
Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198

MATERIALS RESEARCH LABORATORY ACADEMIC STAFF

The staff is grouped according to their departmental affiliations. The number of tenure and non-tenure senior scientists directly associated with the Laboratory is 50. The number of Research Associates (a Research Associate is normally a Ph.D. scientist whose term of appointment does not exceed two years) is 21; we also have five postdoctoral fellows on the MRL staff. There are 118 graduate students with appointments as Research Assistants. In addition to these students, there are 16 graduate students holding fellowships and 5 teaching assistants who are directly associated with the Laboratory through senior scientists who direct their thesis research.

Department of Ceramic Engineering

Baldoni, J. G., Research Assistant
Bergeron, C. G., Professor
Erensberger, F. M., Visiting Professor
Friedberg, A., Professor
Herron, W., Research Assistant, Ingram-Richardson Corp.
Janecek, J. J., Research Assistant
Kumar, A. H., Research Assistant
Leedecke, C., PPG Industries Fellow
Petty, D., Research Assistant
Rita, R. A., Research Assistant
Shukla, V. N., Research Assistant
Wirtz, G. P., Associate Professor
Yu, C. J., Research Assistant

Department of Chemical Engineering

Drickamer, H. G., Professor (joint appointment with Chemistry)
Fanselow, D. L., Research Assistant
Hockert, E. N., U. I. Fellow and Teaching Assistant
Hook, J., III, Research Assistant
House, G. L., MMM Company Research Assistant
Moon, S. H., Research Assistant
Okamoto, B., Research Assistant and Proctor Gamble Fellow
Tyner, C. E., Shell Co. Foundation Fellow
Wilson, D. G., NSF-G Fellow
Woracek, D. L., Research Assistant

Department of Chemistry

Alms, G. P., Research Associate
Atwood, J., Research Assistant
Bertucci, S., Research Assistant
Brown, T. L., Professor
Byers, B., Research Assistant
Burnham, A., Teaching Assistant
Campbell, J. H. Research Assistant
Chabay, I., Postdoc Biophysical Trainee
Curtin, D. Y., Professor
Davis, J., NSF Fellow
Delker, G., Research Assistant
Desiraju, G., Teaching Assistant
Durana, S., Research Associate, NSF
Fieselmann, B., Teaching Assistant
Flygare, W. H., Professor
Gierke, T. D., Research Assistant
Hartford, S., NSF Trainee
Hsieh, N. Y., Research Associate
Ireland, P., U. of I. Fellow
Ishizu, Y., Japanese National Student
Jonas, J., Professor
Jungst, R., Research Assistant
Lee, Y. K., Research Assistant
Lin, C. T., Research Associate
Mink, R. I., Teaching Assistant
Parkhurst, H. J., Research Assistant
Puckett, S. A., Research Assistant
Raj, T., Biophysical Trainee
Schultz, A. J., Research Associate
Sekutowski, D., NSF Fellow
Stucky, G. D., Professor
Sweany, R., NSF Fellow
Tachikawa, M., U. of I. Fellow
Walczak, M., Research Assistant
Wilbur, D. J., Research Assistant

Department of Electrical Engineering

Campbell, J. C., IBM Postdoctoral Fellow
Chie, C. L., Research Assistant
Hennig, F., Research Assistant
Hitchens, W. R., Research Assistant
Holonyak, N., Jr., Professor

Lee, M. H., Research Assistant
Lee, S. H., Visiting Research Assistant Professor
Lo, T. Y., Research Assistant
Ludowise, M. J., Research Assistant
Neugroschel, A., Visiting Research Associate
Sah, C. T., Professor (joint appointment with Physics)
Shiue, C. C., Research Assistant
Wang, C. T., Visiting Research Assistant Professor
Wright, P. D., Research Assistant

Department of Geology

Holder, J. T., Assistant Professor
Lee, S., Research Assistant

Department of Metallurgy and Mining Engineering

Abbott, R., Industrial Student
Altstetter, C. J., Professor
Asselin, G. P., Research Assistant
Au, J. J., Research Assistant
Au, Y. K., Research Assistant
Beck, P. A., Professor
Bhowal, P. R., Research Assistant
Birnbaum, H. K., Professor
Cassidy, M. P., Research Assistant
Chakravorty, S., Research Assistant
Fluhr, C. P., Research Assistant
Fraser, H. L., Assistant Professor
Gerk, A. P., Graduate Student
Jones, I. P., Visiting Research Professor
Keiser, J. R., Research Associate
Koch, G. H., Research Assistant
Kulkarni, S., Research Assistant
Labun, L. C., Research Assistant
Lecocq, P. L., Research Assistant
Levis, R. W., Research Assistant
Mattas, R. F., Research Assistant
Metzger, M., Professor
Nelson, J. L., Research Assistant
Pollock, E. L., IBM Postdoc Fellow
Pugh, N., Professor
Rowland, T. J., Professor

Schroeder, T. A., Research Assistant
Shah, D. M., Research Assistant
Shalvoy, R. S., Research Assistant
Shull, R. D., Research Assistant
Steckel, G. L., Research Assistant
Tong, H. C., Research Assistant Professor
Tortorelli, P. F., Research Assistant
Tustison, R. W., Research Assistant
Wayman, C. M., Professor
Wert, C. A., Professor
Yen, A. C., Research Assistant
Zaluzec, N. J., Research Assistant
Zapp, P. E., Research Assistant

Department of Physics

Aadsen, D. R., Research Assistant
Aldrich, C., III, Research Assistant and NSF Fellow
Allen, P. C., Research Assistant
Anderson, A. C., Professor
Aton, T. J., Research Assistant and IBM Fellow
Barbulesco, N. K., Research Assistant
Bardeen, J., Professor
Baym, G., Professor
Bensel, J. P., Research Associate
Berker, T. D., Research Assistant
Bethin, J. R., Research Assistant
Bhatt, R., Research Assistant and University Fellow
Bhattacharyya, P., Research Associate
Birtcher, R. C., Research Assistant
Bowen, M., Research Assistant
Bray, J. W., Research Assistant
Breger, L., University Assistant
Christy, D. J., Research Assistant
Chu, K. C., Research Assistant
Clemans, J. E., Research Assistant
Craven, R. A., Research Associate
Crawford, R. K., Assistant Professor
Crues, J. V., Research Assistant
DePasquali, G., Research Assistant Professor
Devaney, P., Research Assistant
Dow, J. D., Professor
Drotning, W. D., Research Assistant

Fauchier, J. F, Research Assistant
Field, R. A., Research Assistant and University Fellow
Fish, G. E., Research Assistant
Flynn, C. P., Professor
Folinsbee, J. T., Research Assistant
Follstaedt, D. M., Research Assistant
Fote, A. A., Research Associate
Franceschetti, D., Research Associate
Gallagher, D., Research Assistant
Ginsberg, D. M., Professor
Granato, A. V., Professor
Griffin, E. L., Research Assistant
Guse, M. P., Research Assistant
Halasa, N., Research Associate
Hall, K. M., Research Assistant
Handler, P., Professor (joint appointment with Electrical Engineering)
Hardy, W. H., Research Assistant
Heald, S. M., Research Assistant
Herman, R. M., Research Assistant
Herrick, R. C., Research Assistant
Hertz, W., Research Associate
Hockett, R. S., Research Assistant
Holy, J. A., Research Assistant
Hsu, C. S., Research Assistant
Isaac, R. D., Research Assistant
Jackson, M. S., Research Assistant
Johnson, M. W., Research Assistant
Joncich, D. M., Teaching Assistant
Klein, M. V., Professor
Koehler, J. S., Professor
Kolber, M., Teaching Assistant
Kunz, A. Barry, Associate Professor
Layton, R. P., Research Assistant
Lazarus, D., Professor
Long, J. P., Research Assistant
Macrander, A. T., Research Assistant
Mapother, D. E., Professor
Marchand, R., Research Assistant
Maurer, R. J., Professor
McMillan, W., Professor
Meyer, R. J., Research Assistant
Meyer, S., Research Associate
Miniscalco, W., Research Assistant
Mitchell, J. L., Research Assistant
Mochel, J. M., Associate Professor

O'Hara, S. G., Research Associate
Paalanen, M., Fellow
Papp, E., Research Assistant Professor
Phelps, D. J., Research Assistant
Pines, D., Professor
Pollock, E. E., IBM Postdoc Fellow
Rascoe, D. L., Research Assistant
Read, D. T., Research Assistant
Rehn, L. E., Research Assistant
Rutledge, J. E., Research Assistant
Salamon, M. B., Associate Professor
Schaffman, M. J., Research Assistant
Schwarz, R. B., Research Associate
Sears, M. P., Research Assistant
Sellers, G. J., Research Assistant
Simmons, R. O., Professor
Simons, D., Research Associate
Slichter, C. P., Professor
Smith, D., Research Assistant
Smith, L. N., Research Assistant
Smith, R. A., Research Associate
Stakelon, T. E., Research Assistant
Stapleton, H. J., Professor
Tai, P., Research Associate
Tilton, R. A., II, Research Assistant
Wallat, R. J., Research Assistant
Weiss, J. D., Research Assistant
Whalley, L. R., Research Assistant
Williams, W. S., Professor (joint appointment with Ceramic Engineering)
Wozniak, W., Research Associate
Zaitlin, M. P., Research Assistant and NSF-G Fellow
Ziraps, V., Soviet Exchange Scholar

MATERIALS RESEARCH LABORATORY

PROFESSIONAL STAFF

Judith Baker, B.A.
Assistant Research Chemist

Richard J. Blattner, M.S.
Research Chemist

Charles A. Evans, Jr., Ph.D.
Senior Research Chemist

Russell F. Marshall, Ph.D.
Research Engineer

Virginia Metze
Research Computer Programmer

Connie Silber, B.A.
Assistant Research Chemist

Peter Williams, Ph.D.
Research Chemist

John B. Woodhouse, B.A.
Research Microprobe Analyst

MATERIALS RESEARCH LABORATORY PUBLICATIONS

July 1, 1973 - June 30, 1974

NSF-Supported Publications

Experimental Research on the Properties of Materials at Very Low Temperatures

Principal Investigator: A. C. Anderson

A. C. Anderson, "Low-Noise ac Bridge for Resistance Thermometry at Low Temperature," Review of Scientific Instruments 44, 1475-1477 (1973). Supported by the National Science Foundation under Grant GH-33634

A. C. Anderson "Refrigeration and Thermometry Below 1 K," Applications of Cryogenic Technology (Scholium, New York, 1973) Vol. 5, p. 144. Supported by the National Science Foundation under Grant GH-33634.

A. C. Anderson and R. E. Peterson, "Transport of Heat Between Electrons and Phonons in Copper Below 0.2 K," physics status solidi b, 56, 243 (1973). Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract DAHC-15-73-G10.

J. T. Folinsbee and A. C. Anderson, "Anomalous Kapitza Resistance to Solid Helium," Physical Review Letters 31, 1580-1581 (1973). Supported by the National Science Foundation under Grant GH-33634.

R. E. Peterson and A. C. Anderson, "The Kapitza Thermal Boundary Resistance," Journal of Low Temperature Physics 11, 639-665 (1973). Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract DAHC-15-73-G10

G. J. Sellers, A. C. Anderson, and H. K. Birnbaum, "The Anomalous Heat Capacity of Superconducting Niobium," Physics Letters 44A, 173-174 (1973). Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

Theory of the Condensed State of Matter

Principal Investigator: John Bardeen

David Allender, James Bray, and John Bardeen, "A Reply on Comment of Inkson and Anderson on 'Model for an Exciton Mechanism of Superconductivity'," Physical Review B8, 4433 (1973). Supported by the National Science Foundation under Grant GH-33634.

David Allender, J. W. Bray, and John Bardeen, "Theory of Fluctuation Superconductivity from Electron-Phonon Interactions in Psuedo-One-Dimensional Systems," Physical Review B9, 119-129 (1974). Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Army Research Office (Durham) DA-HC04-69-C-0007.

John Bardeen, "Electron-Phonon Interaction and Superconductivity," Cooperative Phenomena, edited by H. Haken and M. Wagner (Springer-Verlag, Berlin, 1973), pp. 63-78. Supported by the National Science Foundation under Grant GH-33634.

John Bardeen, "Superconducting Fluctuations in One-Dimensional Organic Solids," Solid State Communications 13, 357-359 (1973). Supported by the National Science Foundation under Grant GH-33634 and by the U. S. Army Research Office (Durham) under Contract DA-HC04-69-C-0007.

R. J. Meyer and W. L. McMillan, "A Simple Molecular Theory of the Smectic C, B and H Phases," Physical Review B9, 899-906 (1974). Supported by the National Science Foundation under Grant GH-33634.

Nucleation and Crystal Growth in Simple Glass Systems

Principal Investigator: C. G. Bergeron

H. S. A. Kumar and C. G. Bergeron, "Crystal Growth Mechanisms of $Na_2B_4O_7$ and PbB_4O_7 from Their Undercooled Melts," Journal of Crystal Growth 22, 58-60 (1974). Supported by the National Science Foundation under Grant GH-33634.

Suzanne R. Nagel and C. G. Bergeron, "Crystallization of $Na_2B_4O_7$ from Its Melt," Journal of the American Ceramic Society 57, 129-132 (1974). Supported by the National Science Foundation under Grant GH-33634, by the NDEA Title IV Fellowships, and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221.

Nuclear Quadrupole Resonance and Spectroscopic Studies

Principal Investigator: T. L. Brown

Thomas E. Boyd and Theodore L. Brown, "Cobalt-59 Nuclear Quadrupole Resonance Spectra of Phosphine and Phosphite Substituted Cobalt Carbonyl Compounds," Inorganic Chemistry 13, 422 (1974). Supported by the National Science Foundation under Grants GH-33634, GP-6396X, and GP-30256X.

Theodore L. Brown, "The Chemistry of Metallic Elements in the Ionosphere and Mesosphere," Chemical Reviews 73, 645-667 (1973). Supported by the National Science Foundation under Grants GH-33634 and GP-30256X.

William D. Covey and Theodore L. Brown, "A Kinetic Study of Amine Substitution in $Mc(CO)_5$(Amine) Complexes," Inorganic Chemistry 12, 2820 (1973). Supported by the National Science Foundation under Grants GH-33634 and GP-30256X, and by the Advanced Research Projects Agency under Contract DAHC-15-73-G10.

Randolph J. Guschl and Theodore L. Brown, "Comparative Study of Base Interactions with Three Methylatocobalt (III) Chelate Complexes," Inorganic Chemistry 12, 2815 (1973). Supported by the National Science Foundation under Grants GH-33634 and GP-30256X, and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221.

Randolph J. Guschl, Raymond S. Stewart, and Theodore L. Brown, "Solvent and Alkyl Substituent Effects on the Kinetics of Base Exchange in Alkylbis (dimethylglyoximato) Cobalt (III)-Trimethylphosphite Complexes," Inorganic Chemistry 13, 417 (1974). Supported by the National Science Foundation under Grants GH-33634 and GP-30256X.

Robert A. LaRossa and Theodore L. Brown, "Cobalt-59 Nuclear Quadrupole and Nuclear Magnetic Resonance Spectra of Cobaloximes," Journal of the American Chemical Society 96, 2072 (1974). Supported by the National Science Foundation under Grants GH-33634 and GP-30256X.

Reactions of Crystalline Organic Compounds in the Solid State

Principal Investigator: D. Y. Curtin

David Y. Curtin, "Stereo Pair Drawings of Crystal Structures Prepared by a Desk Calculator-Computer," Journal of Chemical Education 50, 775-778 (1973). Supported by the National Science Foundation under Grants GH-33634 and GP-34545X, and by the Advanced Research Projects Agency under Contract HC-15-73-G10.

Iain C. Paul and David Y. Curtin, "Thermally Induced Organic Reactions in the Solid State," Accounts of Chemical Research 6, 217-225 (1973). Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract HC-15-73-G10, by the Hoffman LaRoche Foundation, and by the National Institute of Health.

Electron-Phonon Interactions in Simple Metals

Principal Investigator: J. D. Dow

John D. Dow, "Effects of Final-state Interactions on Modulation Spectra of Semiconductors," Surface Science 37, 786-803 (1973). Supported by the National Science Foundation under Grant GH-33634.

John D. Dow, "Screening-enhanced Optical Absorption and the Search for M_3 Critical-points," Physical Review Letters 30, 903-906 (1973). Supported by the National Science Foundation under Grant GH-33634.

John D. Dow, "Compatibility Relationships for X-ray Threshold Shapes," Physical Review Letters 31, 1132-1135 (1973). Supported by the National Science Foundation under Grant GH-33634.

John D. Dow, John E. Robinson, and Thomas R. Carver, "The Mahan Soft X-ray Anomaly in Lithium: Relationship to the Knight Shift," Physical Review Letters 31, 759-762 (1973). Supported by the National Science Foundation under Grant GH-33634, AFOSR (Illinois), by the Atomic Energy Commission (Argonne), and by NSF (Princeton).

John D. Dow and D. L. Smith, "The Role of the Cut-off Energy in Tests of the X-ray Threshold Theory," physica status solidi (b) 63, (1974). Supported by the National Science Foundation under Grants GH-33634 and GH-39132.

John D. Dow, Darryl Lyle Smith, and Frank L. Lederman, "Acceptor-to-Band Transitions in Semiconductors: Photoluminescence, Exponential Absorption Edges, and Final-State Interactions," Physical Review B8, 4612-4626 (1973). Supported by the National Science Foundation under Grant GH-33634.

John D. Dow and Bernd F. Sonntag, "X-ray Edges of Simple Metals: Dependence on Electron Density," Physical Review Letters 31, 1461-1463 (1973). Supported by the National Science Foundation under Grants GH-33634 and GH-39132.

Jess Fauchier and John D. Dow, "An Analytic Approach to the Hydrogen Stark Effect in Weak, Strong, and Ultra-strong Fields," Physical Review A9, 98-107 (1973). Supported by the National Science Foundation under Grant GH-33634.

D. L. Smith and John D. Dow, "Divergent Enhancement of Forbidden X-ray Edges by Lattice Vibrations," Physical Review B9, 2509-2512 (1974). Supported by the National Science Foundation under Grants GH-33634 and GH-39132.

Mass Spectroscopy, Spectrochemistry Research

Principal Investigator: C. A. Evans, Jr.

D. K. Bakale, B. N. Colby, C. A. Evans, Jr., and J. B. Woodhouse, "Reduction of Spectral Interferences in Ion Probe Mass Spectrometry," Proceedings of the 8th National Meeting of the Electron Probe Analysis Society of America, New Orleans, pp. 7A-7D (1973). Supported by the National Science Foundation under Grants GH-33634 and GP-33273, and by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

C. A. Evans, Jr., "Ion Probe Mass Spectrometry: Overview," Thin Solid Films 19, 11-19 (1973). Supported by the National Science Foundation under Grants GH-33634 and GP-33273.

C. A. Evans, Jr., "Secondary Ion Mass Spectrometry - The Ion Probe," Proceedings of the Tutorial Session of the 8th National Meeting of the Electron Probe Analysis Society of America, New Orleans, pp. 29-72 (1973). Supported by the National Science Foundation under Grants GH-33634 and GP-33273.

D. Natusch, R. Davison, R. E. Lamb, J. R. Wallace, and C. A. Evans, Jr., "Trace Metals in Airborne Particles," Proceedings of the Third Clean Air Congress, Dusseldorf, C12-14 (1973). Supported by the National Science Foundation under Grants GH-33634 and GI-31605.

D. F. S. Natusch, J. R. Wallace, and C. A. Evans, Jr., "Toxic Trace Elements: Preferential Concentration in Respirable Particles," Science 183, 202-204 (1974). Supported by the National Science Foundation under Grants GH-33634 and GI-31605.

Electronic Structure of Metallic Alloys

Principal Investigator: C. P. Flynn

C. P. Flynn, "Configurational Energies of High-Valence Impurities Dissolved in Metals," Physical Review B4, 1984-1986 (1974). Supported by the National Science Foundation under Grant GH-33634.

C. P. Flynn, "Effect of Electronic Correlations in the X-ray Edge and Recoil Problems," Physical Review Letters 32, 1058 (1974). Supported by the National Science Foundation under Grant GH-33634.

C. P. Flynn and J. A. Rigert, "Impurity Diamagnetism in Metals," Physical Review B7, 3656-3671 (1973). Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency.

R. A. Tilton, D. J. Phelps, and C. P. Flynn, "Optical Absorption Threshold in Dilute Alkali Metal-Rare Gas Alloys," Physical Review Letters 32, 1006 (1974). Supported by the National Science Foundation under Grant GH-33634.

Experimental Studies of Superconductors

Principal Investigator: D. M. Ginsberg

D. M. Ginsberg, "The Electromagnetic Surface Resistance of a Superconducting Aluminum Alloy," Physical Review B8, 2358-2359 (1973). Supported by the National Science Foundation under Grants GH-33634 and GP-28996.

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Principal Investigator: J. M. Mochel

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Principal Investigator: H. J. Stapleton

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Principal Investigator: G. D. Stucky

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Principal Investigator: W. H. Flygare

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Principal Investigator: Jiri Jonas

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Principal Investigator: Miles V. Klein

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Principal Investigator: W. L. McMillan

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Principal Investigator: C. T. Sah

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Principal Investigator: P. A. Beck

S. Mishra, E. J. Hayes, R. Tustison, and P. A. Beck, "Magnetism in Ni-Cu and Co-Re Solid Solutions," Proceedings of the International Conference on Disordered Metallic Systems, Strasbourg, France, 1973, Journal de Physique 35, C4-194 (1974). Also supported by the National Science Foundation (Non-MRL).

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Principal Investigator: H. K. Birnbaum

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Principal Investigator: R. O. Simmons

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Principal Investigator: C. P. Slichter

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Solid State Phase Transformations and Thin Films

Principal Investigator: C. M. Wayman

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Principal Investigator: C. A. Wert

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Principal Investigator: W. S. Williams

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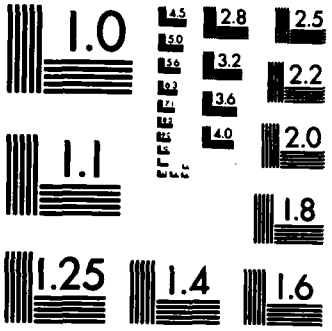

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PH.D DISSERTATIONS

July 1, 1973 - June 30, 1974

Joe Charles Campbell (N. Holonyak, Jr., Adviser), "Indium Gallium Arsenide and Indium Phosphide Injection Lasers and Radiative Recombination in Nitrogen-Zinc-Doped Gallium Arsenide Phosphide," October 1973. Supported by the Advanced Research Projects Agency under Contract HC-15-67-C-0221, by the National Science Foundation under Grants GK-18960 and GH-33771, by the University Industrial Affiliates Program, Night Vision Lab DAAK-02-73-C-0076, and by JSEP DAAB-07-67-C0199.

V. C. K. Chiu (H. G. Drickamer, Adviser), "High Pressure Studies on Mixed Valence Systems," October 1973. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

Peter Wehner Deutsch (A. Barry Kunz, Adviser), "Optical Properties of Simple Molecules," October 1973. Supported by the National Science Foundation under Grant GH-33634 and by the Advanced Research Projects Agency under Contract HC-15-67-C-0221.

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Jess F. Fauchier II (John D. Dow, Adviser), "Topics in the Theory of Condensed Matter: Electron Field Emission, Field Ionization, and Ethane Catalysis," June 1974. Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, and by AFOSR.

Elliott Galetin Flowers, Jr. (G. Baym, Adviser), "Neutrino Emission and Pion Condensation in Dense Matter. Part I. Neutrino Pair Emission in Dense Matter: A Many Body Approach. Part II. Pion Condensation in Nuclear and Neutron Star Matter," October 1973. Supported by the National Science Foundation.

Alvin Phillip Gerk (W. S. Williams, Adviser), "Friction in Intrinsic and N-Type Germanium and Silicon," February 1974. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

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Robert Anthony LaRossa (T. L. Brown, Adviser), "Nuclear Quadrupole Resonance Studies of Cobalt (III) Complexes," October 1973. Supported by the National Science Foundation under Grant GH-33634.

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Albert Migliori (D. M. Ginsberg, Adviser), "Electron Thermal Conductivity of Thin Superconducting Films in Metallic Contact - The Proximity Effect," October 1973. Supported by the National Science Foundation under Grants GH-33634 and GP-28996.

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Sokrates Theodore Pantelides (C. T. Sah, Adviser), "Theory of Point-Imperfection States in Semiconductors," June 1973. Supported by the National Science Foundation under Grant GH-33634, by the Advanced Research Projects Agency under Contract DAHC-15-73-G10, by AFOSR-71-2067, and by U. of I. Grad. Fellowship.

Cheryl Deckert Pribula (T. L. Brown, Adviser), "Spectroscopic Studies of Penta-Coordinate Organometallic Complexes," October 1973. Supported by the National Science Foundation under Grant GH-33634.

Lynn Eduard Rehn (J. Holder and A. V. Granato, Advisers), "Contributions from Point Defects to the Elastic Constants of Copper," February 1974. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the National Science Foundation under Grant GH-33634.

Raymond Marvin Roop (J. S. Koehler, Adviser), "Effects of Electron Irradiation on P-Type Germanium at Liquid Helium Temperatures Using AC Hopping Conductivity," October 1973. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the U. S. Army Research Office (Durham).

Reginald Rutherford III (M. Wortis, Adviser), "Energy Density Correlation in the Three-Dimensional Ising Model," June 1973. Supported by the Advanced Research Projects Agency and by the National Science Foundation.

Mary Ellen Phelen Switzer (T. L. Brown, Adviser), "The Reactivity and Magnetochemistry of Selected Metallocenes," October 1973. Supported by the National Science Foundation.

Yu Wang (G. Stucky, Adviser), "Structural and Bonding Properties of Small Ring Compounds," October 1973. Supported by the National Science Foundation under Grant GH-33634.

John Shi Sun Wei (F. C. Brown, Adviser), "Polaron Transport in Silver Bromide," February 1974. Supported by the National Science Foundation and by the U. S. Army Research Office (Durham).

Jonathan David Weiss (D. Lazarus, Adviser), "The Pressure Dependence of the Thermoelectric Power of Sodium Between 5°K and 14°K," February 1974. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

Lawrence Robert Whalley (C. P. Slichter, Adviser), "Electric Field Gradients in Copper Alloys," February 1974. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

Andrew Chien-Chong Yen (T. J. Rowland, Adviser), "A Study of Precipitation in Copper +13 Atomic Percent Beryllium by Nuclear Magnetic Resonance and Field Ion Microscopy," June 1974. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

Richard Paul Zerger (G. Stucky, Adviser), "Bonding and Stereochemical Studies of Group IA and IIA Organometallic Compounds," October 1973. Supported by the National Science Foundation under Grants GH-33634 and GP-31016X and by the Advanced Research Projects Agency.

M. S. THESES

July 1, 1973 - June 30, 1974

(This list does not include M. S. degrees for which written theses were not required).

Roeland J. Ansems (C. G. Bergeron, Adviser), "Crystallization in Fiberglass Compositions," January 1974. Supported by the National Science Foundation under Grant GH-33634 and by Australian Consolidated Industries Fiberglass Ltd.

Christian Paul Fluhr (C. A. Wert, Adviser), "An Electron Microscopy Study of Carbide Precipitation in a Vanadium-Titanium Alloy," May 1974. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

Terrence Alan Schroeder (C. M. Wayman, Adviser), "Shape Memory Behavior and Mechanical Characteristics of Some Copper Zinc Alloys," June 1974. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198 and by the National Science Foundation under Grant GH-36813.

Douglas Wilson (H. G. Drickamer, Adviser), "High Pressure Studies of Anthracene Homologues," June 1973. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

D. L. Woracek (H. G. Drickamer, Adviser), "Effects of Pressure on Alkali Halides Doped with Lead (II), June 1974. Supported by the U. S. Atomic Energy Commission under Contract AT(11-1)-1198.

ADDITIONAL PROJECTS IN MATERIALS SCIENCE

AT THE UNIVERSITY OF ILLINOIS

Carl J. Altstetter, Professor of Physical Metallurgy
Phase Instability During Low-Cycle Fatigue of Steel
U. S. Army Research Office (Durham) Contract DA-ARO-D-31-124-73-G43

Ansel C. Anderson, Professor of Physics
A Low Temperature Investigation of Amorphous Dielectrics
National Science Foundation Grant NSF-GH-39135

John Bardeen, Professor of Physics and of Electrical Engineering
Theoretical Problems in Solid State and Low Temperature Physics
U. S. Army Research Office (Durham) Contract DAHC-04-74-C-005

Gordon Baym, Professor of Physics
Properties of Solids and Many Particle Systems
National Science Foundation Grant NSF-GP-40395

Paul A. Beck, Professor of Physical Metallurgy
Study of the Alloys of Transition Metals
National Science Foundation Grant NSF-GH-37568X

Howard K. Birnbaum, Professor of Physical Metallurgy
An Investigation of the Mechanisms of Hydrogen Embrittlement in BCC Metals
U. S. Office of Naval Research Contract ONR-00014-67-A-0305-0020

Theodore L. Brown, Professor of Chemistry
Organometallic Chemistry
National Science Foundation Grant NSF-GP-30256X2

David Y. Curtin, Professor of Chemistry
Reaction Mechanism Studies and Exploratory Organic Chemistry
National Science Foundation Grant NSF-GP-34545X

John D. Dow, Associate Professor of Physics
Theory of Solids and Polyatomic Systems
National Science Foundation Grant NSF-GH-39132

Charles A. Evans, Jr., Senior Research Chemist, Materials Research Laboratory
Ion Microprobe Mass Spectrometry
National Science Foundation Grant NSF-GP-33273

Colin P. Flynn, Professor of Physics
Electronic Structure of Hydrogen in Metals and on Metal Surfaces
U. S. Office of Naval Research Contract N00014-67-A-0305-0027

Willis H. Flygare, Professor of Chemistry
High Resolution Microwave Spectroscopy
National Science Foundation Grant NSF-GP-40668X

Donald M. Ginsberg, Professor of Physics
Properties of Superconductors
National Science Foundation Grant NSF-GH-37980

Andrew V. Granato, Professor of Physics
Defect Interactions in Crystals
National Science Foundation Grant NSF-GH-37907

Nick Holonyak, Jr., Professor of Electrical Engineering
Luminescence and Laser Studies in $In_{1-x}Ga_xP$ (and Related III-V Compounds) in the Near Infrared Spectrum ($0<x\leq 9.25$)
U. S. Army Research Contract DA-AK-02-72-C-0076
Luminescence and Laser Studies in III-V Semiconductors
National Science Foundation Grant NSF-GH-33771

Jiri Jonas, Professor of Chemistry
Nuclear Magnetic Resonance Study of Relaxation Phenomena
National Science Foundation Grant NSF-GP-28268X
High Pressure Nuclear Magnetic Resonance Relaxation Study of Supercritical Dense Fluids
U. S. Air Force Office of Scientific Research AFOSR-72-2286

Miles V. Klein, Professor of Physics
Light Scattering Studies in Insulators, Semiconductors, and Glasses
National Science Foundation Grant NSF-GH-37757

A. Barry Kunz, Associate Professor of Physics
Research in Electronic Structure of Solids
U. S. Air Force AF-F-33615-72-C-1506

Marvin Metzger, Professor of Physical Metallurgy
Film Breakdown and Fitting
U. S. Army Research Office (Durham) Contract DA-HC-04-74-G0016

Jack M. Mochel, Associate Professor of Physics
Third Sound Resonance and Phonon Interference in Thin Helium Films
National Science Foundation Grant NSF-GH-37892

David Pines, Professor of Physics
Astrophysical Applications of Microscopic Many-Body Theory
National Science Foundation Grant NSF-GP-37485X

E. Neville Pugh, Professor of Metallurgy
The Mechanism of Stress-Corrosion Cracking
U. S. Army Research Office (Durham) Contract DA-HC-04-G0127

Chih-Tang Sah, Professor of Electrical Engineering and of Physics
Silicon Extrinsic Detectors
U. S. Air Force AF-19628-72-C-0199
Circuit Models of Semiconductors Devices
National Science Foundation Grant NSF-GK-30283
Interface and Bulk Phenomena in Solid State Components which have Characteristics Useful in Air Force Systems
U.S. Air Force Office of Scientific Research Contract AF-OSR-71-2067

Myron B. Salamon, Associate Professor of Physics
Comparative Critical Point Measurements
National Science Foundation Grant NSF GH-33750

Cameron Satterthwaite, Professor of Physics
Studies of Superconductivity in Metal-Hydrogen Systems
National Science Foundation Grant NSF-GH-33381

Galen D. Stucky, Professor of Inorganic Chemistry
Structural Properties of Group I, II, and III Organometallic Compounds
National Science Foundation Grant NSF-GP-31016X

Marvin C. Wayman, Professor of Metallurgical Engineering
Martensitic Transformations in Iron Alloys
U. S. Army Research Office (Durham) Contract DA-HC-04-74-G0134
Properties and Characteristics of Shape Memory ('Marmen') Materials
National Science Foundation Grant NSF GH-36813

Charles A. Wert, Professor of Physical Metallurgy
Measurements of the Dependence of the Elastic Constants of Structural Materials Upon Hydrogen Additions
National Science Foundation Grant NSF-GH-41045


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